

Spring 1991

# A comparative analysis of the efficacy of zero-order, first-order and Monod kinetic models in representing raw aerobic biodegradation data

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A Comparative Analysis of the Efficacy of Zero-Order, First-Order  
and Monod Kinetic Models in Representing Raw Aerobic  
Biodegradation Data

by

Andrew I. Bakun

NJIT Masters Thesis  
Department: Chemical Engineering  
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Date: June 17, 1991



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## 1. Abstract

A total of 148 raw aerobic biodegradation data sets from batch and continuous stirred-tank reactors were extracted from the open literature and previous NJIT MS theses. Kinetic analysis of each of these data sets was performed with respect to the following commonly-used empirical models: (1) zero-order, (2) first-order, and (3) Monod. Two constant-biomass versions of each model were evaluated; one in which  $S_0$  (i.e., the boundary condition for substrate concentration at time equal to zero) was assumed to be equal to the measured value of the initial substrate concentration and the other in which  $S_0$  was treated as a regressable parameter. Where adequate biomass concentration data were available, variable-biomass versions of each model, in which  $S_0$  was assumed to be equal to the initial substrate concentration, were also evaluated. Each data set was categorized within one of nine different biodegradation data types and discussed with respect to the advantages and disadvantages of each model evaluated for the given data type. Model selection recommendations were given for each data type.

A theoretical analysis of the effects of variations in raw biodegradation data on the corresponding regression results was performed for the constant- and variable-biomass models. The effects of random experimental error, number of data points, sampling regularity and substrate concentration range were evaluated. The impact of erroneous models on reactor sizing was also demonstrated.

## 2. Introduction

Chemical reactors assume many forms in a variety of industries. Regardless of the type of application, they are typically the focal point of a given process. Their proper design is of critical importance to the overall performance and economics of a process. This is just as true for wastewater treatment plants as it is for any conventional chemical or petrochemical process plant.

Of primary importance to the efficient design and operation of a chemical or biochemical reactor is a kinetic model which is consistent with physical reality. Biochemical reactions, which rely on the metabolic pathways of microorganisms, are inherently much more difficult to mechanistically model than conventional chemical reactions. No universal theoretical equation currently exists which can reasonably represent a cell's metabolic processes. As a result, academia and industry alike typically resort to empirical equations such as the zero-order, first-order, and Monod to model biochemical reactions. Their choice of which model to use in a given situation, however, has tended to be haphazard and lacking in scientific consistency.

The purpose of this thesis is to address this issue and to provide a foundation for the selection of empirical models for aerobic biodegradation reactions. A complementary objective of this thesis is to elucidate the relationship between the quantity/quality of experimental data and model selection, which, in turn, should provide further insight into the critical aspects of experimental data measurement.

### 3. Scope

This thesis is best viewed as being composed of two parts. The first part involves an extensive review of the literature for raw aerobic biodegradation data. The retrieved data are fit to constant-biomass versions of zero-order, first-order, and Monod kinetic models using linear regression analysis. Two variations of each model type are investigated. One in which regression is forced through the initial value of substrate concentration and the other in which initial substrate concentration is treated as an additional regressable parameter. Variable biomass versions of the zero-order, first-order, and Monod kinetic models are also evaluated using linear regression analysis for the cases in which adequate biomass concentration data are available.

The purpose of this first part of the thesis is two-fold: (1) to provide insight into the different aerobic biodegradation data types (i.e., substrate concentration vs. time curves) attained in industrial and academic research under a wide range of experimental conditions (e.g., substrate/biomass types and concentrations, temperature, and pH), and (2) to determine the advantages/disadvantages of each model for a given data type. Both batch reactor and continuous stirred-tank reactor aerobic biodegradation data are considered.

The second part of the thesis entails a theoretical analysis of the effects of variations in raw biodegradation data on the corresponding regression results for the constant- and variable-biomass models. The effects of experimental error, number of data points, sampling regularity and substrate concentration range are evaluated. This analysis will provide additional insight into the applicability of the above models in different situations, as well as give a better understanding of the critical aspects of experimental data measurement with respect to kinetic analysis.



#### 4. Theory

In biological wastewater treatment, bacteria and other micro-organisms break down and metabolize the soluble and colloidal organic material thereby reducing the BOD (biochemical oxygen demand) and COD (chemical oxygen demand) to acceptable levels. At the molecular level, this is an extremely complex process; substrate is absorbed by the bacterial cell along with other essential nutrients (e.g., N, P, oxygen, minerals, and cofactors), wherein it is acted upon by a myriad of enzymes as part of the cell's metabolism, ultimately yielding various amounts of cell growth and carbon dioxide or soluble nondegradable residue. Theoretical models are, as yet, unable to adequately represent the microscopic phenomena which occur. As a result, empirical equations are typically used to model the relationship between substrate concentration and time without regard for the actual mechanisms taking place.

The zero-order, first-order, and Monod equations are the most commonly used (i.e., by academia and industry) empirical models in the kinetic analysis of aerobic biodegradation data. Assuming that the organic substrate is the limiting reagent (i.e., all other nutrients are supplied in excess) and that no diffusion or mass-transfer limitations exist (i.e., the reaction is kinetically controlled), the order of the biodegradation reaction will depend on the concentration of substrate relative to that of the bacterial biocatalyst. At high

ratios of substrate to biocatalyst, the biodegradation rate will be limited by bacterial concentration and should be independent of substrate concentration (i.e., zero-order). At low ratios, substrate concentration is limiting relative to bacterial concentration and the biodegradation rate becomes proportional to substrate concentration (i.e., first-order). For ratios spanning both the zero-order and first-order regions, the shifting order kinetics of the Monod equation<sup>1</sup> will apply.

The mathematical derivation of the kinetic expressions used as a basis for the linear regression of biodegradation rate constants from batch reactor and continuous stirred-tank reactor data are presented in detail in Appendices A and B, respectively. Table 1 summarizes the integrated kinetic expressions used for batch reactor data analysis. The parameters in these equations (i.e., a, b, and c) are determined by linear regression using the method of least-squares analysis (refer to Appendix A, page A-17).

The above integral treatment of substrate concentration, S, versus time, t, batch reactor data is used in this thesis as opposed to the more empirical differential treatment for the following reasons: (1) the inherent difficulty in accurately determining the differential,  $dS/dt$ , either analytically (by first fitting the data with a polynomial function) or graphically, and (2) the inability of the differential approach to fit anything other than nth-order kinetics (i.e., analysis of Monod equations is not possible).

Table 1  
Batch Reactor Kinetic Expressions

| <u>Model</u>              | <u>Integrated Kinetic Expression*</u>  |
|---------------------------|--|
| Constant Biomass:         |  |
| Zero-order (1-parameter)  | $t = (1/k)(S_0 - S)$ $= (a)(x)$  |
| Zero-order (2-parameter)  | $t = (-1/k)S + (S_0/k)$ $= (a)x + (b)$   |
| First-order (1-parameter) | $t = (1/k)(\ln(S_0/S))$ $= (a)(x)$   |
| First-order (2-parameter) | $t = (-1/k)\ln S + ((\ln S_0)/k)$ $= (a)x + (b)$   |
| Monod (2-parameter)       | $t = (K/k)\ln(S_0/S) + (1/k)(S_0 - S)$ $= (a)x + (b)z$   |
| Monod (3-parameter)       | $t = (-K/k)\ln S + (-1/k)S + ((K/k)\ln S_0 + (S_0/k))$ $= (a)x + (b)z + (c)$   |
| Variable Biomass:         |  |
| Zero-order (1-parameter)  | $t = (1/koY_c)(\ln((Bo + Y_c S_0 - Y_c S)/Bo))$ $= (a)(x)$   |
| First-order (1-parameter) | $t = (-1/(ko(Bo + Y_c S_0)))(\ln(BoS/((Bo + Y_c S_0 - Y_c S)S)))$ $= (a)(x)$   |
| Monod (2-parameter)       | $t = (K/(ko(Bo + Y_c S_0)))(\ln((Bo + Y_c S_0 - Y_c S)S/(BoS)))$ $= (a)(x)$ $+ (1/(koY_c))(\ln((Bo + Y_c S_0 - Y_c S)/Bo))$ $+ (b)(z)$ |

\* a, b, and c are regressable parameters; t, x, and z are given data (refer to Appendix A, page A-3, for clarification of nomenclature).

In the least-squares analyses performed in this thesis, minimization of model error is performed with respect to the independent variable,  $t$ , and not the dependent variable,  $S$ . This is done because all of the models being considered are not linear and explicit with respect to  $S$ , whereas they are with respect to  $t$ . The statistic  $\Sigma(t-t_{\text{calc}})^2$  will, therefore, provide a common basis of comparison between models.

The kinetic expression that minimizes the sum of the squares of the discrepancies between model predictions and measured values is the one with the highest probability of being correct. The statistic  $\Sigma(t-t_{\text{calc}})^2$  alone does not, however, indicate whether a given model is a good fit; it only tells which of the models considered is statistically best. A model can be considered a good fit to a set of data if the experimental points are normally distributed around the predicted curve due to random error during measurement. This can be readily detected graphically in a plot of substrate concentration,  $S$ , versus time showing both experimental data and the predicted curves. The calculation of  $S$  as a function of time is straightforward (once the parameters have been regressed) for the zero- and first-order models since these expressions are explicit with respect to  $S$ . The Monod models, however, are not explicit in  $S$  and therefore require trial-and-error solution of the variable. The Newton-Raphson method is used here for this purpose (refer to Appendix A, page A-23).

It should be noted that slightly different results would be obtained if the regression analyses were performed relative to the dependent variable,  $S$ , rather than the independent variable,  $t$ . In a plot of  $S$  versus  $t$ , regression with respect to  $t$  will minimize the error in the horizontal direction between the given model and data, whereas regression with respect to  $S$  would minimize the error in the vertical direction. While the standard convention is to perform regression with respect to the dependent variable and plot it on the ordinate versus the independent variable, it was not followed here. Regression with respect to  $t$  in this thesis facilitates a straightforward statistical comparison between the models being investigated. The graphical results, however, are presented in the standard manner of  $S$  versus  $t$  for ease of interpretation. This fact should be remembered when reviewing results since the errors between the predicted curves and experimental data will be minimized in the horizontal direction with respect to  $t$ , as opposed to the more common approach of error minimization in the vertical direction relative to the dependent variable,  $S$ .

Table 2 summarizes the kinetic expressions used for continuous stirred-tank reactor analysis. The regression of kinetic parameters and subsequent analysis of results are performed in the same manner as the batch reactor data analysis. The calculation of  $S$  as a function of time for the Monod models, however, is slightly simpler, requiring solution by quadratic formula only.

Sample calculations for the regression of kinetic parameters from batch reactor data are shown for both the constant- and variable-biomass models in Appendix C. Also included are printouts of LOTUS 123 spreadsheets which were developed to facilitate these tedious calculations (refer to page C-16). Calculations for the regression of kinetic parameters from continuous stirred-tank reactor data are methodically analogous to that shown for the batch reactor and, hence, sample calculations for them are not included.

It should be noted that the higher-parameter versions of the variable-biomass models (i.e., where  $S_0$  is treated as a regressable parameter) were not considered as part of the base group of models studied in this thesis. Analysis of these models requires non-linear regression techniques which are outside the main scope of this work.

Table 2

CSTR Kinetic Expressions

| <u>Model</u>              | <u>Kinetic Expression*</u>   |
|---------------------------|--|
| Constant Biomass:         |  |
| Zero-order (1-parameter)  | $(V/Q) = (1/k)(S_i - S_e)$ $= (a)(x)$  |
| Zero-order (2-parameter)  | $(V/Q) = (-1/k)S_e + (S_i/k)$ $= (a)x + (b)$   |
| First-order (1-parameter) | $(V/Q) = (1/k)((S_i - S_e)/S_e)$ $= (a)(x)$  |
| First-order (2-parameter) | $(V/Q) = (S_i/k)(1/S_e) + (-1/k)$ $= (a)(x) + (b)$   |
| Monod (2-parameter)       | $(V/Q) = (K/k)((S_i - S_e)/S_e) + (1/k)(S_i - S_e)$ $= (a)(x) + (b)(z)$  |
| Monod (3-parameter)       | $(V/Q) = (S_i K/k)(1/S_e) + (-1/k)S_e + ((S_i - K)/k)$ $= (a)(x) + (b)z + (c)$   |
| Variable Biomass:         |  |
| Zero-order (1-parameter)  | $(V/Q) = (1/k_o)((S_i - S_e)/(B_i + Y_c(S_i - S_e)))$ $= (a)(x)$   |
| First-order (1-parameter) | $(V/Q) = (1/k_o)((S_i - S_e)/((B_i + Y_c(S_i - S_e))S_e))$ $= (a)(x)$  |
| Monod (2-parameter)       | $(V/Q) = (K/k_o)((S_i - S_e)/((B_i + Y_c(S_i - S_e))S_e))$ $= (a)(x) + (1/k_o)((S_i - S_e)/(B_i + Y_c(S_i - S_e)))$ $+ (b)(z)$ |

\* a, b, and c are regressable parameters; (V/Q), x, and z are given data (refer to Appendix B, page B-3, for clarification of nomenclature).

## 5. Literature Search

An extensive search of the scientific literature was conducted for raw aerobic biodegradation data resulting in the extraction of 63 sets of data from 24 articles encompassing 8 different trade journals. Batch and CSTR data from both mixed-culture and single-culture systems were considered, providing each set consisted of a minimum of 4 points. A listing of the literature references used is given in Appendix D (page D-3), while a breakdown by data type is provided in the following table:

| <u>System</u>  | <u>Number of Data Sets*</u> |                  |
|----------------|-----------------------------|------------------|
|                | <u>Batch Reactor Data</u>   | <u>CSTR Data</u> |
| Mixed Culture  | 39(7)                       | 4(4)             |
| Single Culture | 16(6)                       | 4(4)             |

\*Values in parentheses refer to the number of data sets for which variable-biomass concentration data were available.

In addition to the above literature data, 85 sets of raw aerobic biodegradation data were extracted from a total of six previous New Jersey Institute of Technology MS Theses (refer to Appendix E, page E-3, for a listing). All of the data sets were for batch-reactor activated-sludge systems, while 18 of the total included variable-biomass concentration data.

All in all, a broad base of data involving 27 different substrates was compiled for this study.



The treatment of the above-mentioned data with respect to kinetic analysis and modelling by the respective authors varied dramatically. Of the 24 articles used, 9 performed no kinetic analysis at all (references 7, 9, 14, 16, 17, 21-24 in Appendix D, pages D-3 through D-5). These papers were concerned more with the feasibility of biodegradation of specific substrates and the underlying biological mechanisms and metabolic pathways than with modelling of the data. The remaining 15 papers, on the other hand, used a myriad of different equations to model their biodegradation data: zero-order (references 1,4), first-order (references 3, 10, 12, 13, 18), second-order (reference 6), Monod (references 3, 15, 19), modified versions of Monod to account for substrate inhibition (references 2, 8, 11, 15), and more sophisticated mechanistic models (references 5, 15, 20). A lack of consistency in the selection and application of models is readily apparent.

## 6. Discussion of Regression Analysis Results

The raw aerobic biodegradation data extracted from the literature sources and previous New Jersey Institute of Technology MS Theses were regressed using the method of least-squares analysis for the constant- and variable-biomass versions (the latter, where applicable) of the zero-order, first-order, and Monod kinetic models with the results from the data sources being compiled in Appendices D and E, respectively. Both appendices include lists of the relevant references and indices of the results contained therein. The results are presented within the appendices in the form of summary sheets for each raw biodegradation data set studied. Each summary sheet presents the raw data used, the literature reference from which it was extracted, the conditions under which the data were experimentally determined, and the corresponding regression analysis results (i.e., regressed kinetic rate constants and sum-of-the-squares of the errors for each model).

The discussion of the regression analysis results is performed in subsections according to reactor (i.e., batch and CSTR) and culture (i.e., mixed and single species) types. To make the discussion of these results more tractable, the data sets are grouped and discussed according to major trends in biodegradation data type (e.g., zero-order, first-order, Monod, etc.). Anomalies are also noted, along with the capabilities/inabilities of each of the models studied to represent the data. Where applicable, appropriate comparisons and comments are made with respect to kinetic analyses performed in the literature references utilized in this thesis.

### 6.1 Batch Reactor Data--Mixed Culture Systems

The bulk of the raw biodegradation data available in the literature is derived from batch reactors because they are much simpler than continuous reactor systems to set up, run and obtain kinetic data. Furthermore, ideal batch reactor behavior in terms of perfectly-mixed conditions can be, and for the most part is, closely approximated, thereby facilitating a relatively straightforward and reliable kinetic analysis. Of the 148 data sets studied in this thesis, 140 are for batch reactor systems.

Discussion of batch reactor biodegradation data within this thesis is subdivided according to the general categories of mixed- and single-culture systems to provide some insight into any differences which may be evident between the two cases with respect to kinetic modelling. Most of the batch reactor data sets studied here (i.e., 124 out of 140) utilized mixed cultures. The high percentage of biodegradation studies performed in the literature utilizing mixed cultures directly follows from the fact that virtually all wastewater treatment facilities and the environment, in general, operate under such conditions.

The raw biodegradation data types discussed in the following subsections are for the most part some variation of one of the two curves shown in Figure 1 providing that the substrate is limiting and that the reaction is kinetically controlled (i.e., diffusion and mass-transfer resistances are negligible). Curve 1 is for the case of constant biomass while Curve 2 is for the variable-biomass case with

Figure 1

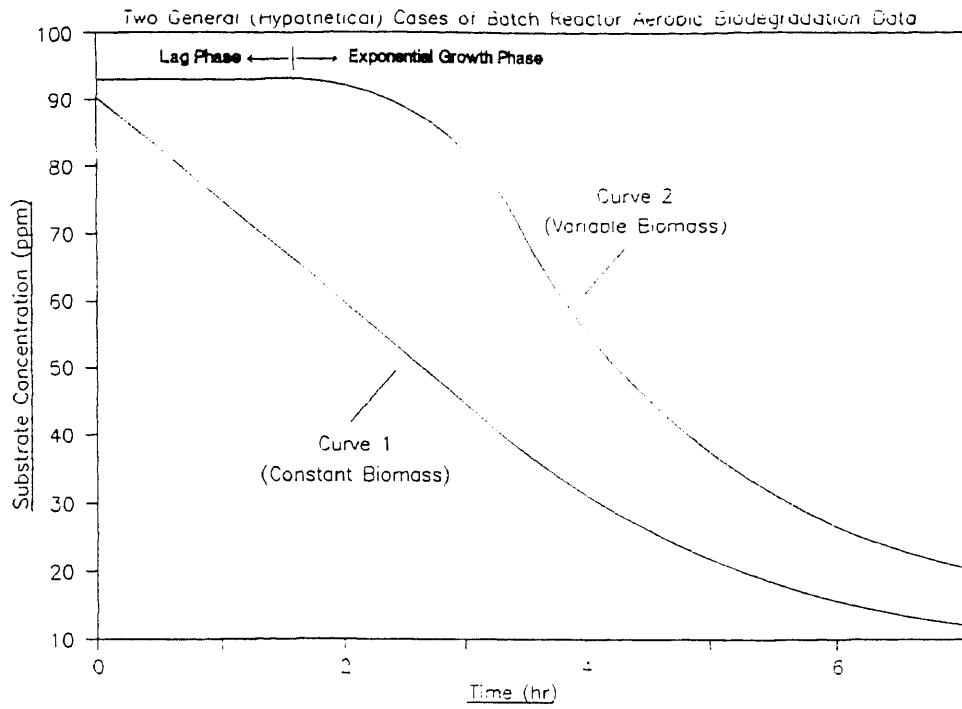
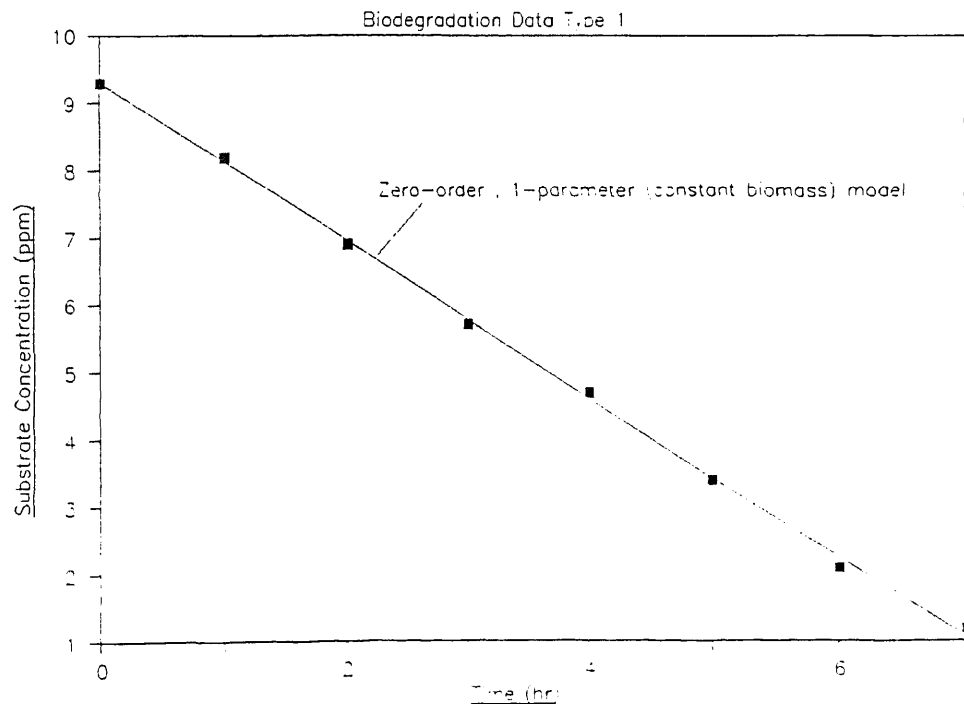


Figure 2



Source: Naik Thesis (data set #8B) ; refer to page E-50

both the lag phase and exponential growth phase for a typical bacterial culture being schematically presented. Depending on the portion of either curve over which a given data set is measured, it can be interpreted as being either the constant- or variable-biomass form of the zero-order, first-order or Monod kinetic models. The designation of a given data set as a specific biodegradation data type is not always definitive because of a combination of factors such as experimental error, missing data points, and measurement over ranges intermediate between two different data types.

#### 6.1.1 Data Type 1 (Zero-Order, Constant Biomass)

The first biodegradation data type to be discussed is the zero-order, constant-biomass type presented in Figure 2. The data set shows substrate concentration,  $S$ , to be a linear function of time,  $t$ , with very little data scatter and is well represented by the zero-order, 1-parameter, constant-biomass model. This data type can be expected when  $S$  is high relative to the viable biomass concentration. At first glance, the data in Figure 2 might not be expected to follow zero-order kinetics because of the low  $S$  range (i.e., 1.2-9.3 ppm) covered for an activated sludge system where the total biomass concentration,  $B$ , is high (e.g., typically 2000-5000 ppm). The activated sludge, however, was not acclimated to the substrate and, as such, only a very small proportion of the bacterial population was capable of metabolizing the substrate. It is readily apparent that the prediction of data type cannot be generalized from the values of

S and B alone; knowledge of the population of viable bacteria is also required.

A comparison of the constant-biomass versions of the zero-order, first-order, and Monod kinetic models in representing the data from Figure 2 is presented on page E-80 in terms of the statistics  $\Sigma(t-t_{calc})^2$  and  $\Sigma(S-S_{calc})^2$  (note--the values listed on the summary sheets in Appendices D and E are normalized with the sum-of-the-squares of the error of the relevant parameter being divided by the number of data points used). The former statistic is more pertinent in this study than the latter since the least-squares analyses were all performed with respect to the explicit variable  $t$ , and not  $S$ . The latter statistic is provided for comparison purposes only. In terms of the data shown in Figure 2, the best models based on the statistic  $\Sigma(t-t_{calc})^2$  are, in order: (1) Monod (3-parameter) or M3, (2) Monod (2-parameter) or M2, (3) zero-order (2-parameter) or Z2, (4) zero-order (1-parameter) or Z1, (5) first-order (2-parameter) or F2, and (6) first-order (1-parameter) or F1. The difference between the first four models is minimal with the regressed curves all being virtually identical to that shown in Figure 2. The first-order models, F1 and F2, are statistically and visually much worse (refer to Figure 3).

The Monod model ( $-dS/dt = kS/(K+S)$ ) reduces to zero-order kinetics when  $S \gg K$ , as is the case in Figure 2 with the value of  $k$  being virtually the same for both model types. From a regression

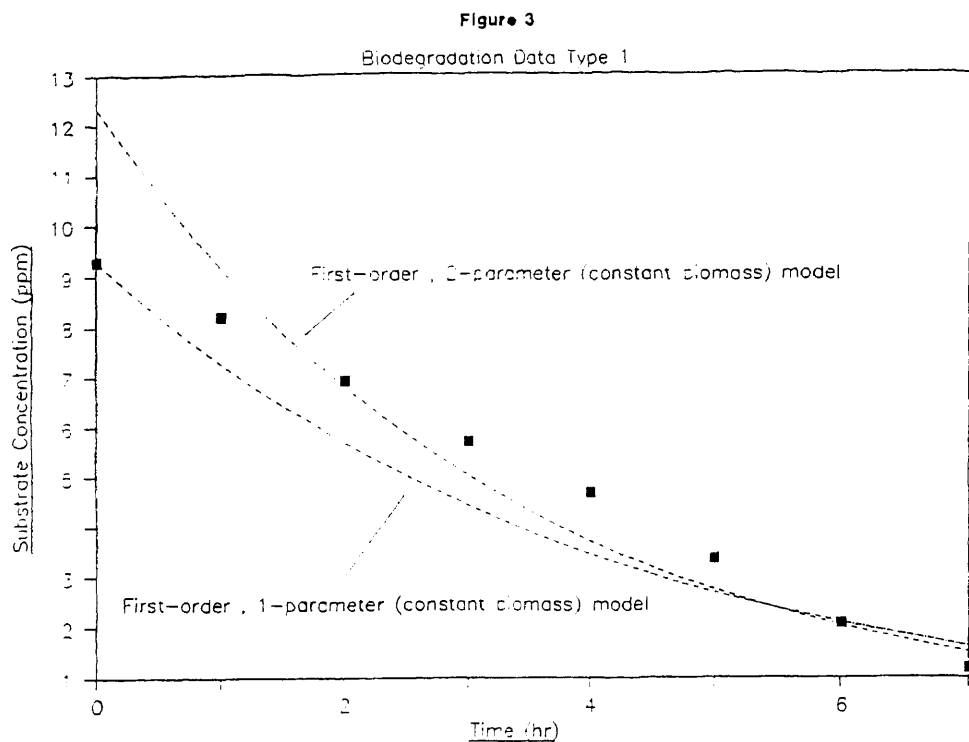
analysis perspective, the Monod model is expected to be statistically better than the zero-order model in representing raw aerobic biodegradation data because of the regressable parameter  $K$  which gives the Monod model an additional degree of freedom in fitting the data. For truly zero-order kinetics with ideal data (i.e., no systematic or random errors of measurement), the two models would yield identical results. But since some degree of experimental error is always present, the Monod model will always be statistically better than the corresponding zero-order model (i.e., M3 vs. Z2 and M2 vs. Z1). In general, the more scatter in the data, the greater the difference expected. In the case of Figure 2, the difference between Monod and zero-order models is small because of the apparent high accuracy of the raw data.

In line with the discussion of the above paragraph, the models which regress for  $S_0$  will yield statistically better results than those which assume  $S_0 = S(t=0)$  because of the extra degree of freedom provided by the additional regressable parameter in the fitting of a model to a given set of data. For ideal data of a given kinetic type (i.e., zero-order, first-order or Monod), the two cases would yield identical results. But for real data with experimental uncertainties, the higher-parameter versions are better with the differences becoming more pronounced as experimental error increases. In the case of Figure 2, the higher-parameter versions of the Monod and zero-order models are only marginally better because of the apparent minimal experimental error present.

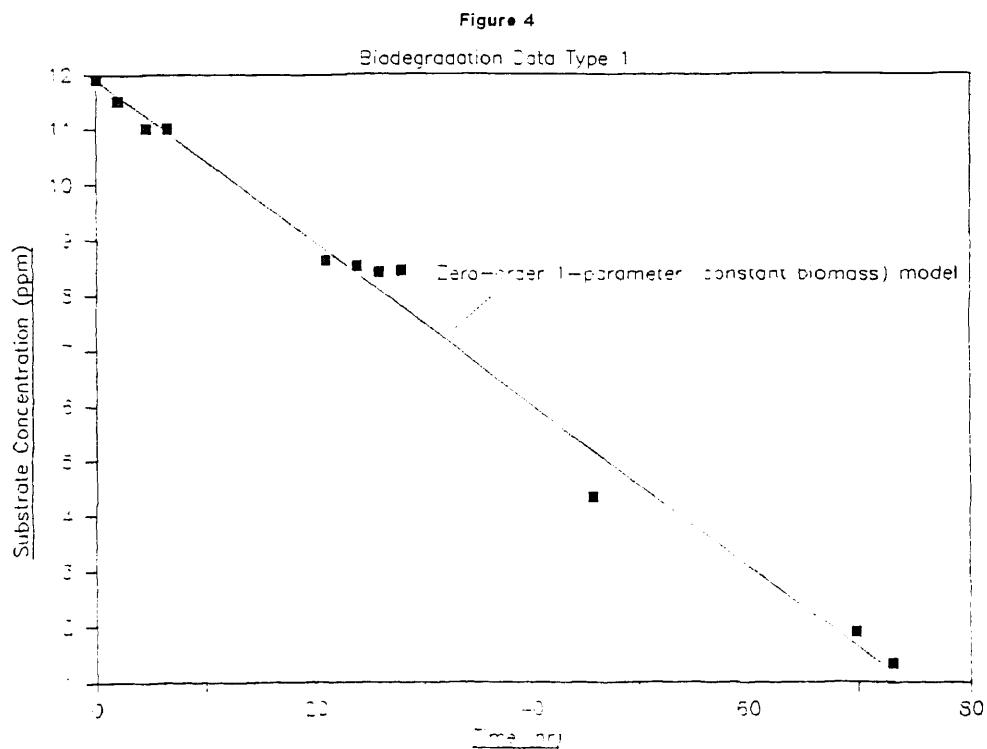
The regressed first-order models for the data shown in Figure 2 are presented in Figure 3. It is apparent that both versions are incorrect representations of reality. The 1-parameter version, F1, fits the initial point  $S_0 = S(t=0)$  and approximates the latter points while underpredicting the rest. The curvature is inherent in the model ( $S = S_0 \exp(-kt)$ ) and the preferential fit of the latter region over the intermediate is attributed to the logarithmic function (i.e.,  $x = \ln(S_0/S)$ ) used in the regression analysis which naturally favors the latter (lower  $S$  value) points (refer to page C-6). The 2-parameter version, F2, also fits the latter points in the same manner and for the same reason, but averages the error over the rest of the data range to minimize  $\sum(t-t_{calc})^2$  by excessively overpredicting  $S_0$ . F2 is statistically better in terms of  $\sum(t-t_{calc})^2$ , as expected, but worse in terms of  $\sum(S-S_{calc})^2$ . Slightly different results would be obtained if the least-squares analyses were performed to minimize the error in  $S$ ; F2 would be visually better with a lower value of  $\sum(S-S_{calc})^2$ , but worse in terms of  $\sum(t-t_{calc})^2$ . In any case, no first-order model could well represent the zero-order kinetics observed in Figure 2.

Another example of biodegradation data type 1 is presented in Figure 4. It is analogous to the data set in Figure 2 in that no first-order effect is apparent even though the  $S$  range is low (i.e., 1.3-11.9 ppm) relative to  $B$  (i.e., 3800-4100 ppm). This is





Source : Naik Thesis (data set #8B) ; refer to page E-80



Source : Gonnabathula Thesis (data set #13) ; refer to page E-25

attributed to the fact that only a very small percentage of the total biomass measured is viable for the substrate in question, 2,6-dichlorophenol, which is reputed to be relatively resistant to bacterial utilization.

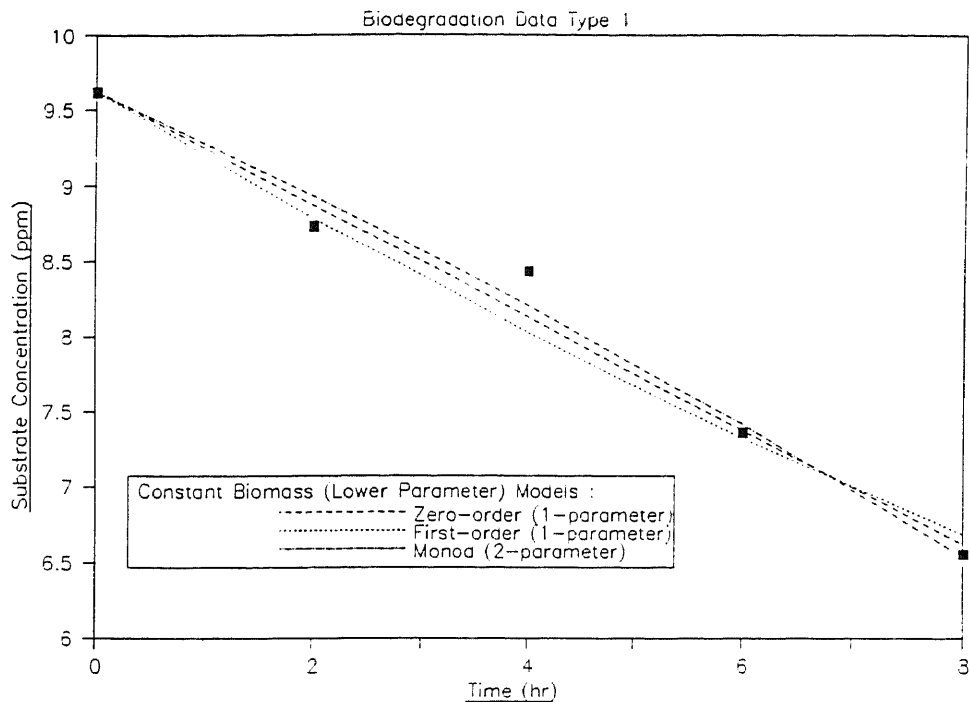
The data set in Figure 4 has an increased amount of scatter compared to that in Figure 2. This increase in data scatter results in a dramatic increase in the average sum-of-the-squares of the error in  $t$  for both the Monod and zero-order models, while having a significantly smaller effect on the first-order models. Although  $\Sigma(t-t_{calc})^2$  is still much higher for the first-order models than for either the zero-order or Monod, it is obvious that model differentiation and, hence, proper model selection becomes more difficult as uncertainties in experimental measurement increase.

Although the data set in Figure 4 shows significantly more scatter than the data set in Figure 2, the regressed curves for Z1, Z2, M2 and M3 all coincide with one another. This is the result of the experimental error in the data being approximately normally distributed around the predicted zero-order curve. The first-order curves are, in effect, identical to those shown in Figure 3 and are therefore not presented nor discussed further here.

Figures 5 and 6 graphically present the results from page E-97 for the lower- and higher-parameter constant-biomass models, respectively. This data appears to be the same type as the previous two sets discussed so far except with a much higher degree of scatter relative to the small S range covered. As mentioned previously, increased scatter makes model differentiation and proper model selection more difficult. Statistically, the sequence of models from best to worst is unchanged from the previous sets. The difference between best and worst (i.e., M3 and F1), however, is much less with Figures 5 and 6 showing all six curves to be reasonable over the S range covered. Extrapolation of any of the models considered outside of the measured range, however, would be extremely risky and ill-advised because of the low level of certainty on which model, if any, is correct; for lower values of S, the errors caused by selection of an incorrect model would be greatly magnified.

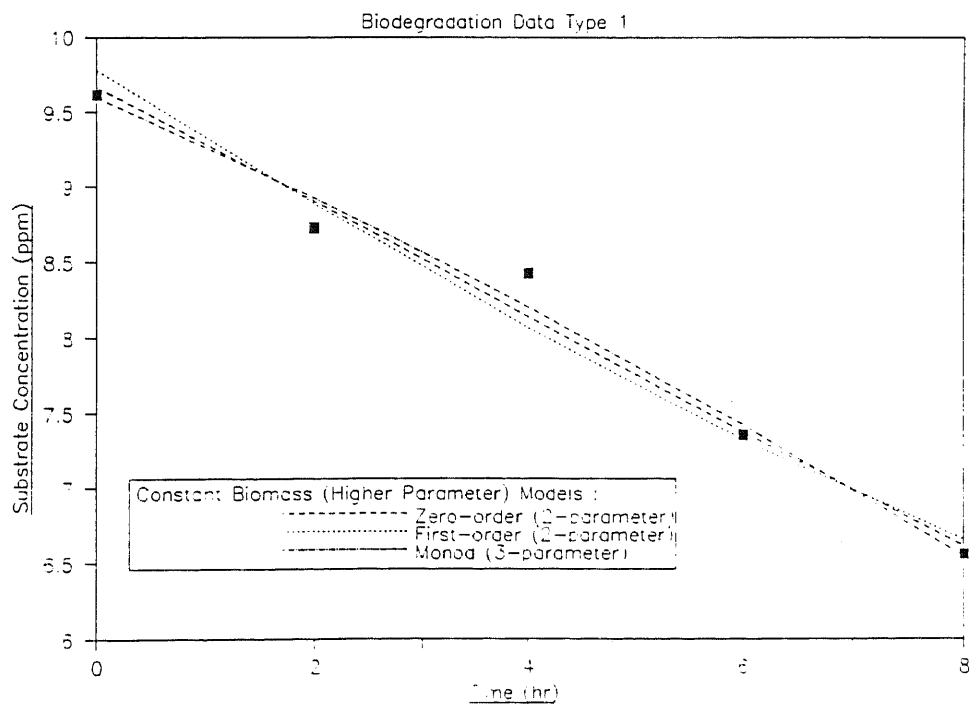
While the Monod models are statistically best (in all cases), the regression results on page E-97 indicate negative values of the kinetic parameter K for both the 2- and 3-parameter versions. A negative value of the rate constant K is physically uninterpretable and nullifies any theoretical basis in the Monod model derived from the Michaelis-Menten relationship<sup>1</sup>. Regression yields a negative value of K because the scatter in the data gives the effect of a slight downward slope. The Monod models minimize  $\sum(t-t_{calc})^2$  by using a

Figure 5



Source : Pak Thesis (data set #4) ; refer to page E-97

Figure 6

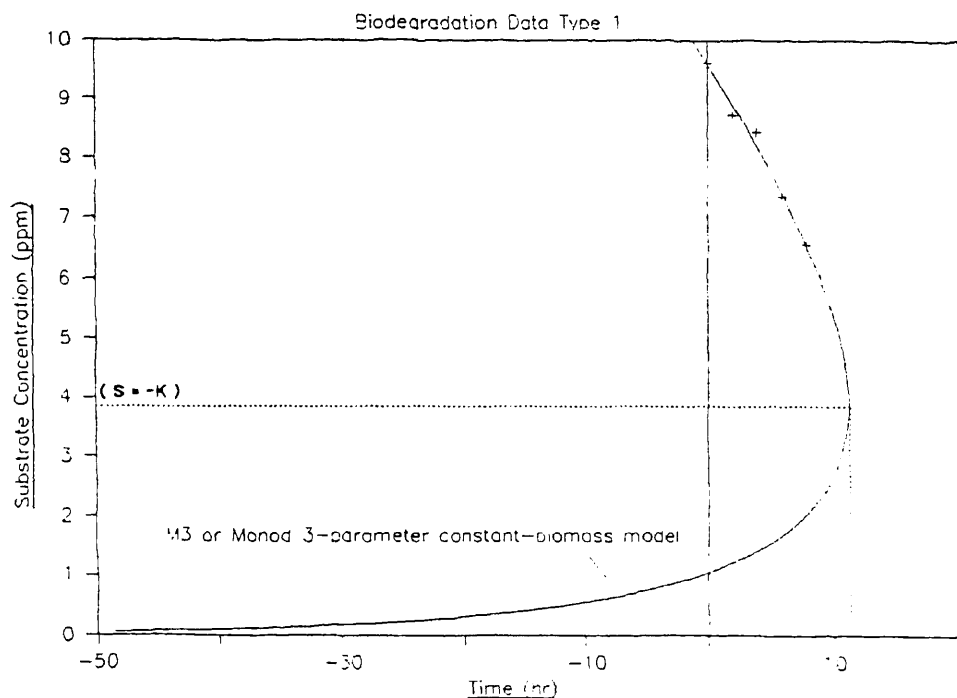


Source : Pak Thesis (data set #4) ; refer to page E-97

negative  $K$  to fit the apparent curvature rather than yielding the conventional first-order curvature obtained with a positive value of  $K$ . While the Monod models in Figures 5 and 6 fit the data over which they were regressed, extrapolation down to  $S$  values approaching the absolute value of  $K$  is not feasible as  $-dS/dt$  goes to infinity (i.e.,  $-dS/dt$  indeterminate at  $S = -K$ ), thereby limiting the practical usefulness of an already theoretically invalid model. This problem is displayed graphically in Figure 7 which shows an expanded version of the predicted M3 curve from Figure 6. The curve doubles back on itself at a value of  $S$  equal to the absolute value of  $K$ .

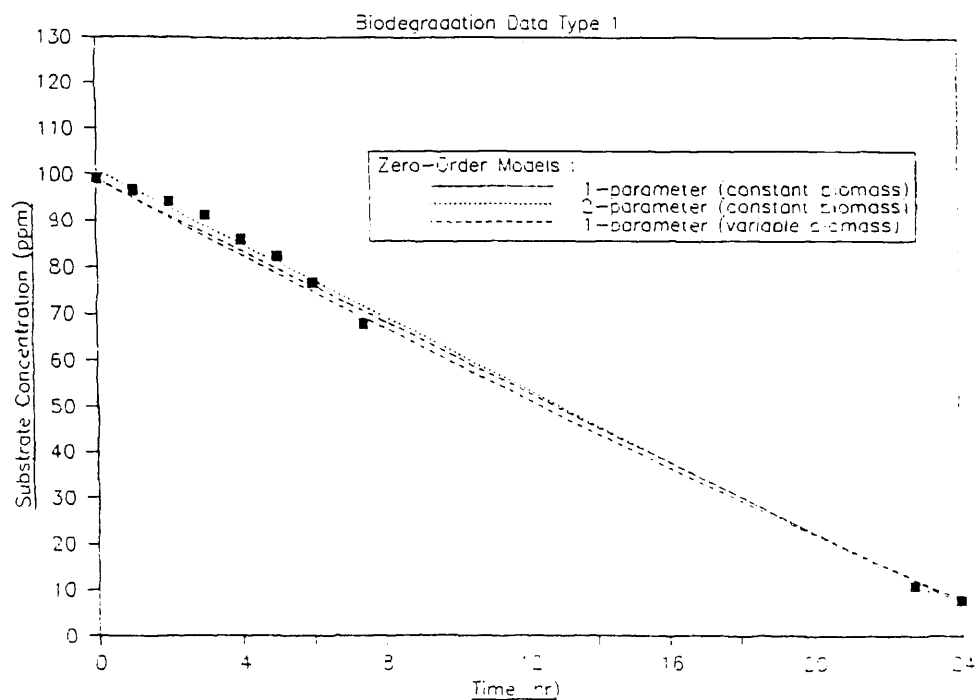
The Monod models have an approximately equal likelihood of regressing negative values for  $K$  as they do positive values for any zero-order kinetic data. The value of  $K$  for the case of zero-order kinetics is dependent solely on the scatter in the data resulting from experimental errors in their measurement and whether the overall set, as a result, is interpreted as having either a slight upward or downward curvature. Because of this problem with the Monod models in representing zero-order kinetics, the zero-order models are, in general, best for interpolating type 1 data even though the Monod are statistically always somewhat better. Extrapolation of the zero-order models below the range in which the kinetic parameters

Figure 7



Source: Pak Thesis (data set #4) ; refer to page E-97

Figure 8

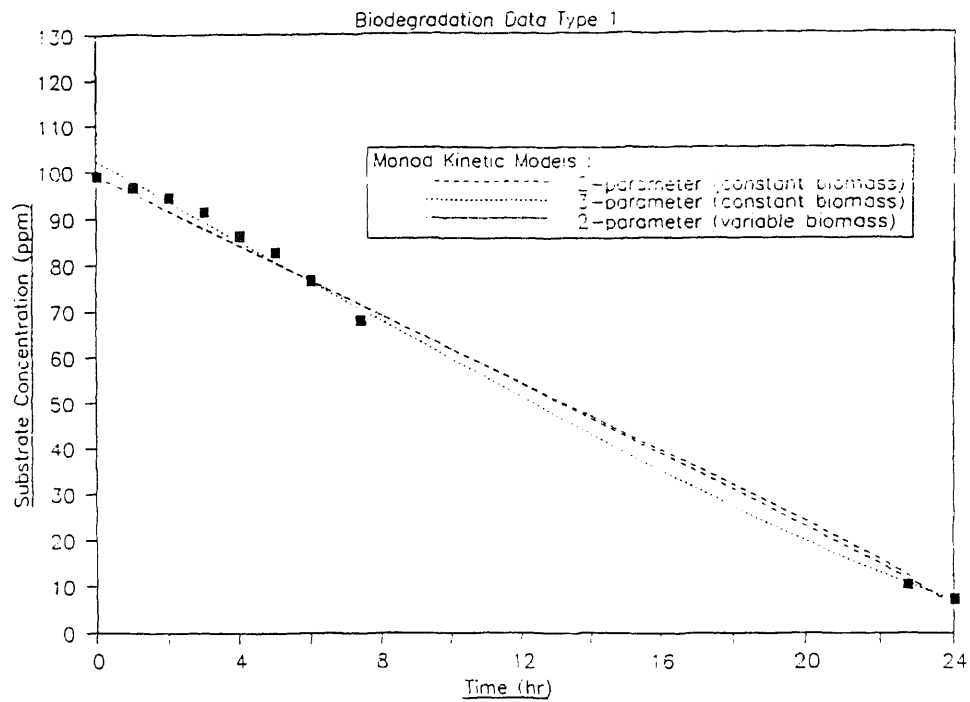


Source: Pak Thesis (data set #9) ; refer to pages E-104 & 105

were regressed, however, is unrealistic since it predicts negative values of  $S$  for  $t > S_0/k$ . In reality, as  $S$  becomes smaller, it will asymptotically approach the  $t$  axis in an infinitely long "tail". Since most pollution problems require removals down to very low levels, final effluent concentrations are generally in the "tail". In such cases, a zero-order model can grossly underpredict the size of the reactor.

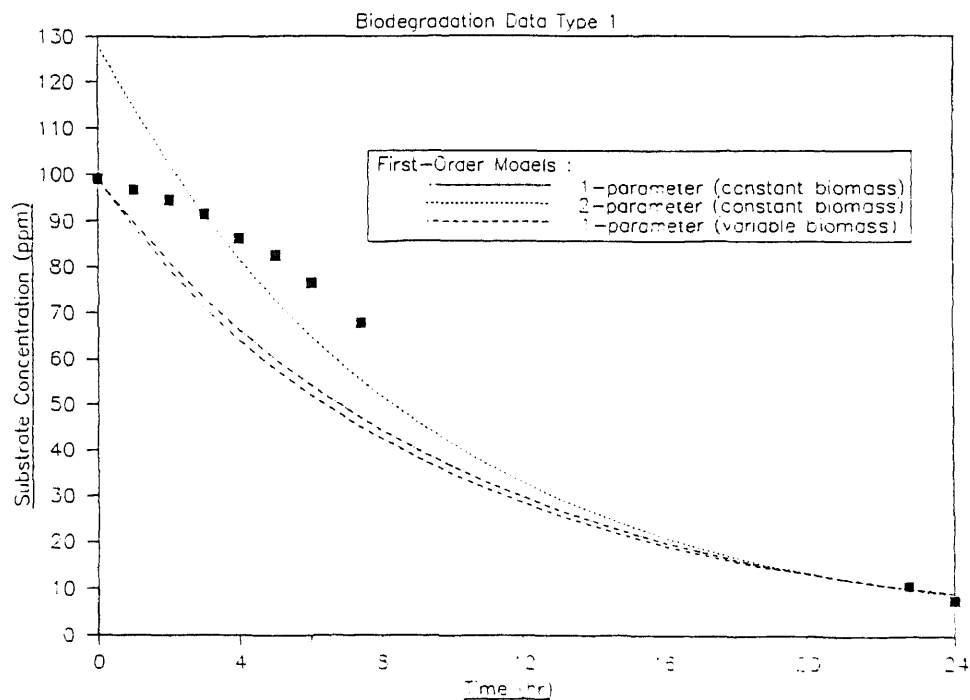
Figures 8-10 graphically represent the regression results summarized on pages E-104 and E-105. Unlike the cases discussed thus far, this system included biomass concentration data which facilitated regression analysis of the variable-biomass kinetic models. The variable-biomass models used in this thesis assume a linear relationship between biomass generated and substrate consumed, with the proportionality constant being designated as the yield coefficient (i.e.,  $Y_c = (B - B_0)/(S_0 - S)$ ). A value between 0 and 1 is typically expected. For this case, however, a negative value of  $Y_c$  was calculated based on raw biomass data with a linear correlation coefficient of 0.86. The reason for the negative value of  $Y_c$  is less likely inaccuracy in the measurement of  $B$  (because of a relatively high correlation coefficient) than the nature of the mixed-culture system itself. If the proportion of bacteria in a mixed-culture system capable of metabolizing a specific substrate is small (as is apparently so in this case), the "total" biomass concentration may decrease due to endogenous respiration while the level of substrate-specific bacterial concentration actually increases. The values of

Figure 9



Source : Pak Thesis (data set #9) ; refer to pages E-104 & 105

Figure 10



Source : Pak Thesis (data set #9) ; refer to pages E-104 & 105



$B_0$  and  $Y_c$  used in the variable-biomass models should be based on measurements of viable, and not total, biomass measurements in order to yield reliable regression results. Unfortunately, such measurements are not easily made for mixed-culture systems. The bulk of the variable biomass data utilized in this thesis is based on the dried weights of insoluble biomass. This method does not differentiate between living and dead cells, let alone viable ones. Pike and Carrington<sup>2</sup> showed that the percentage of total bacteria which are viable in various stages of wastewater treatment operations is typically on the order of only 1 to 3%. Furthermore, "weight" is not as reliable a measure of total biodegradation activity as "number of cells" because of the tendency of cells to fluctuate in size (via the creation/utilization of storage products) with slight changes in the environmental condition of the culture. Regardless of the aforementioned limitations and problems, analysis of the performance of the variable-biomass models in this thesis should provide considerable insight into their sensitivity to  $B_0$  and  $Y_c$ , as well as their applicability and flexibility in different situations.

The best models for the data on pages E-104 and E-105 based on the statistic  $\Sigma(t-t_{calc})^2$  are in order: (1) M3, (2) Z2, (3) M2, (4) Z1, (5) Monod (variable biomass, 2-parameter) or MV, (6) zero-order (variable biomass, 1-parameter) or ZV, (7) F2, (8) F1, and (9) first-order (variable biomass, 1-parameter) or FV. Figures 8, 9 and 10 graphically present the results for the zero-order, Monod and

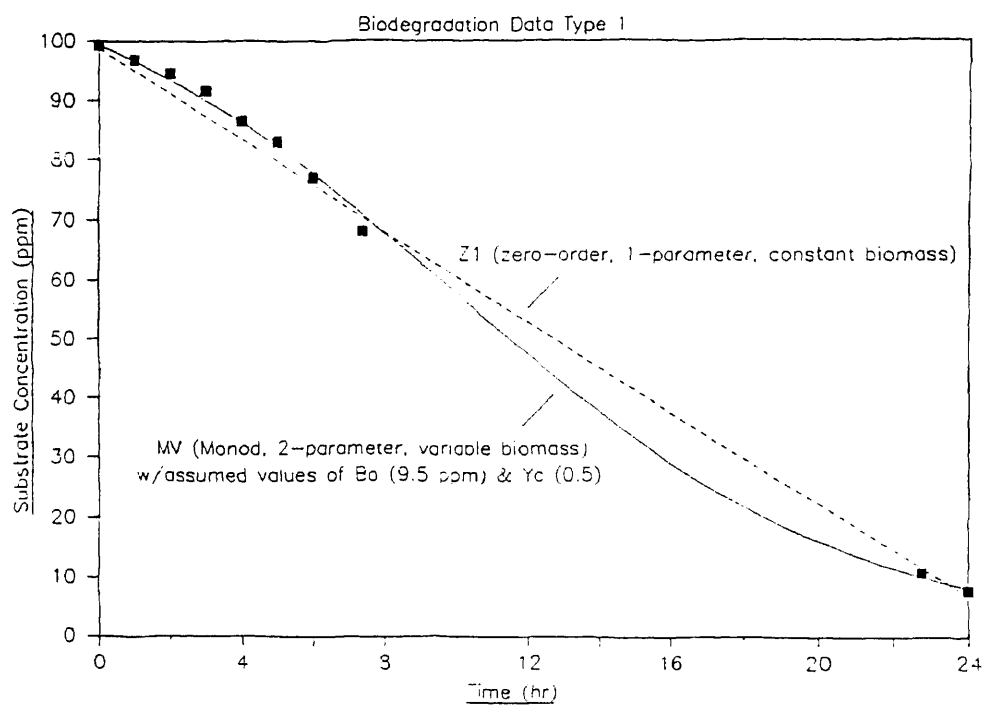
first-order models, respectively. Figures 8 and 9 show all the zero-order and Monod models to be reasonable given the quality/quantity of the data, while Figure 10 shows all the first-order models to be poor. As expected, the models with  $S_0$  as a regressable parameter are better than the corresponding constant-biomass models with  $S_0 = S(t=0)$ . In this case, the higher-parameter zero-order model, Z2, is even statistically better than the lower-parameter Monod, M2. Unexpectedly, the variable-biomass models are all statistically worse than the corresponding constant-biomass versions. With accurate values of  $B_0$  and  $Y_c$ , the variable-biomass models should always be better than or equal to the corresponding lower-parameter constant-biomass versions as a result of the additional parameters representing catalyst concentration. The aforementioned problem with measurement of "total" and not "viable" biomass is the cause of the determination of an erroneous negative value for  $Y_c$  which, in turn, accounts for the reduced performance of the variable-biomass models. Another problem with the measurement of "total" biomass (instead of "viable" biomass) in terms of the variable-biomass models is that the values of  $B$  are often so large that effectively constant-biomass behavior is predicted even when the  $S$  vs.  $t$  data indicate exponential growth. In the case of Figures 8-10, the variable-biomass models, although statistically worse than the corresponding lower-parameter constant-biomass versions (i.e., MV vs. M2, ZV vs. Z1 and FV vs. F1), are only slightly worse because  $B$

decreases by only 15% over the  $S$  range covered thereby closely approximating constant-biomass behavior. Since the variable-biomass curves in Figures 8-10 are so similar to the corresponding constant-biomass curves, detailed discussion of the characteristics of the variable-biomass models and the effect of  $B_0$  and  $Y_c$  upon them is reserved for subsequent examples where the phenomenon of exponential bacterial growth is visually more readily apparent.

Figure 9 shows all 3 versions of the Monod model to be reasonable for the data given. Both M2 and MV, however, yield negative values for  $K$  while M3 regresses a positive  $K$ . The 2-parameter models yield a negative  $K$  because of a slight downward bend in the data when forcing the curves through  $S_0 = S(t=0)$ . When the  $S_0$  restriction is relaxed in the case of M3, the data is interpreted as having a slight upward bend thereby accounting for the positive value of  $K$  being regressed.

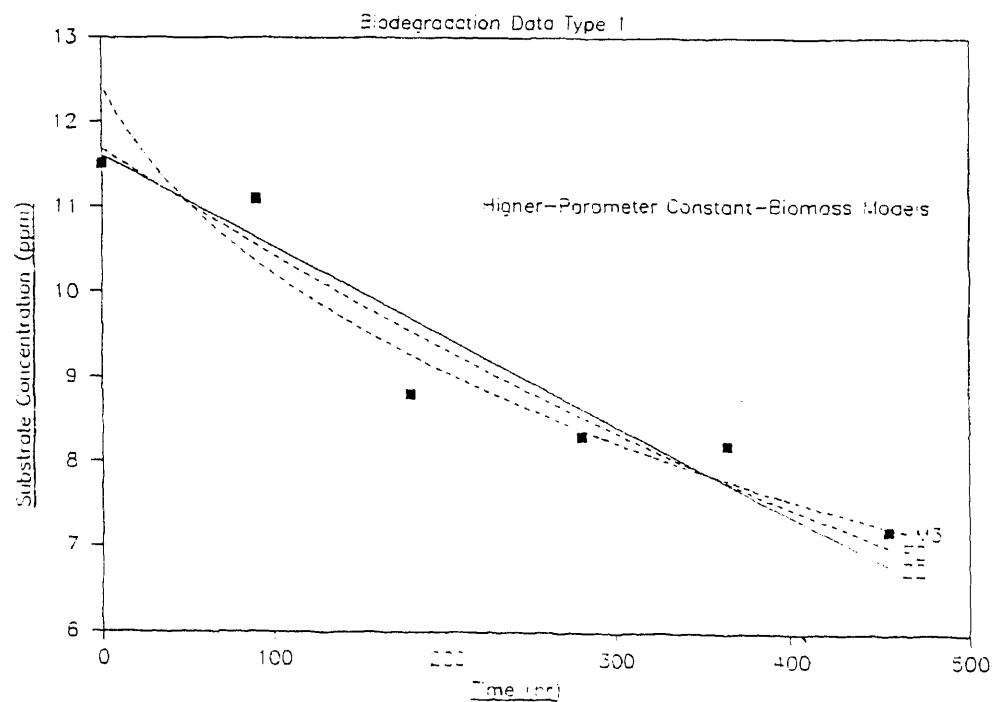
While the data in Figures 8-10 have been interpreted as type 1 (i.e., zero-order, constant biomass), significant uncertainty exists as to whether it is an accurate interpretation because of the missing gap of data between 8 and 24 hours. Figure 11 shows the data and Z1 curve along with a hypothetical MV curve for which values of  $B_0$  and  $Y_c$  were arbitrarily selected so as to provide a good fit of the apparent subtle curvature in the data. The MV curve provides a visually and statistically better fit, and indicates that depiction of this

Figure 11



Source : Pak Thesis (data set #9) ; refer to pages E-104 & 105

Figure 12



Source : Salerno Thesis (data set #1) ; refer to pages E-107 & 108

data set as zero order may likely be incorrect. This case illustrates the necessity of measuring data at frequent intervals over the entire range of interest, when reliable kinetic modelling is desired, in order to reduce the probability of missing critical features of the  $S$  vs.  $t$  curve. Unfortunately, irregularity in data measurement was a common occurrence for the data extracted from the previous NJIT theses, specifically for systems which ran overnight. As a side note, a comparison of the two MV curves in Figures 9 and 11 demonstrate the importance of  $B_0$  and  $Y_c$  accuracy on the performance of the variable-biomass model.

Figure 12 graphically presents the higher-parameter constant-biomass models for the data set shown on page E-107 (the corresponding variable-biomass results are shown on page E-108). This set has a very high degree of data scatter and covers a small  $S$  range thereby making model differentiation impossible (compare  $\Sigma(t-t_{calc})^2$  and  $\Sigma(S-S_{calc})^2$  on pages E-107 and E-108). While this data set is arbitrarily designated as type 1, the Monod models predict curvature in excess of first order for each case (M2 being the only one shown in Figure 12). As a result of the interpretation of the data set by the Monod models as greater than first-order, M2, M3 and MV all regress negative values for the kinetic parameters  $k$  and  $K$ . This phenomenon is discussed in greater detail in later sections where its occurrence is more commonplace.

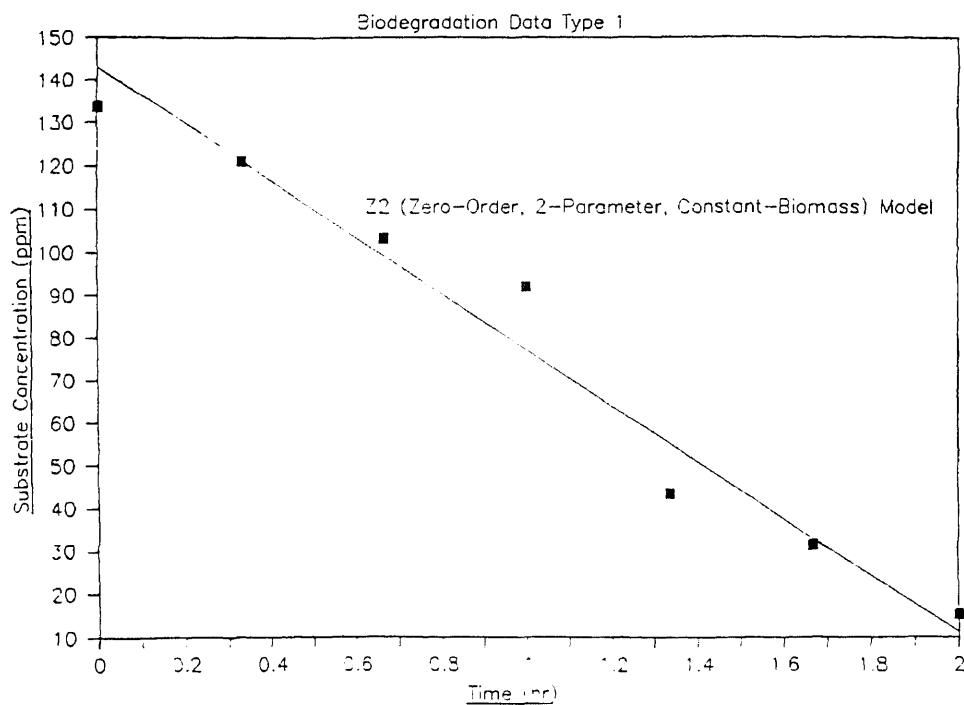
In addition to the 5 data sets discussed thus far, 4 more of the data sets reviewed were interpreted as type 1. Each set of raw data along with the corresponding regressed Z2 curves is presented in Figures 13 and 14. None of these data sets are of good quality. All 4 have a high degree of data scatter while the latter 3 (i.e., those in Figure 14) suffer from missing gaps of data over the range of S studied. The Monod models regress negative values of K for all 4 cases.

#### 6.1.2 Data Type 2 (First-Order, Constant Biomass)

The second aerobic biodegradation data type to be discussed is the first-order, constant-biomass type shown in Figure 15 to be well represented by the F2 curve. Theoretically, first-order kinetics are expected for systems such as this one where the substrate concentration is low (i.e., <10 ppm) relative to biomass concentration (i.e., activated sludge), assuming all other nutrients are supplied in excess and that no mass-transfer limitations exist.

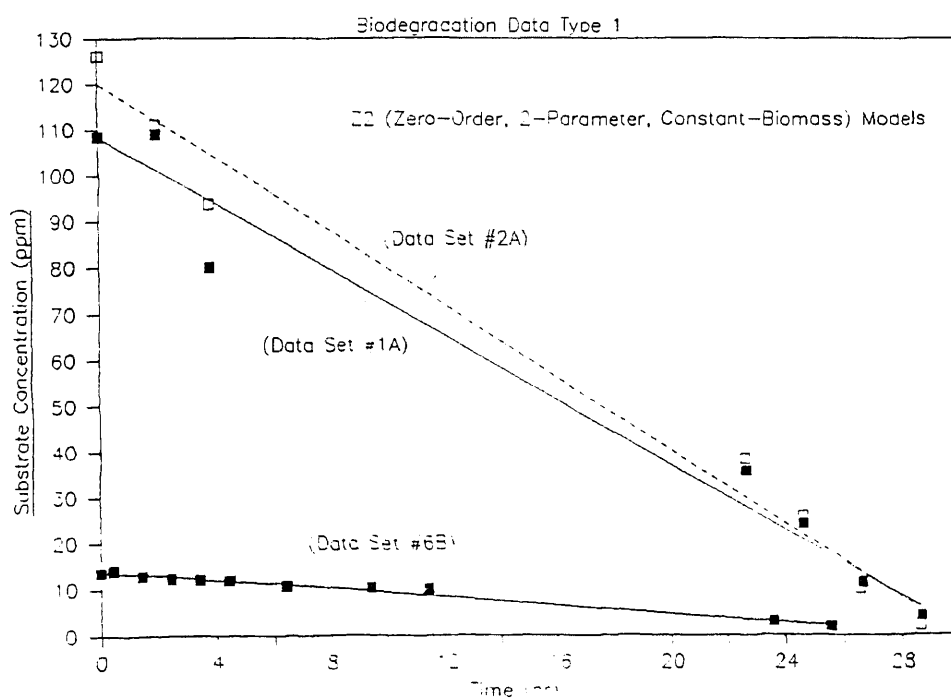
A comparison of the constant-biomass versions of the zero-order, first-order and Monod kinetic models in representing the data shown in Figure 15 is tabulated on page E-65. Statistically, the best models based on minimization of  $\Sigma(t-t_{calc})^2$  are in order: (1) M3, (2) M2, (3) F2, (4) F1, (5) Z2, and (6) Z1. The regressed results for the lower-parameter models are presented graphically in Figure 16. The corresponding higher-parameter models are virtually identical to those shown in Figure 16 (due to minimal data scatter) and are therefore not shown.

Figure 13



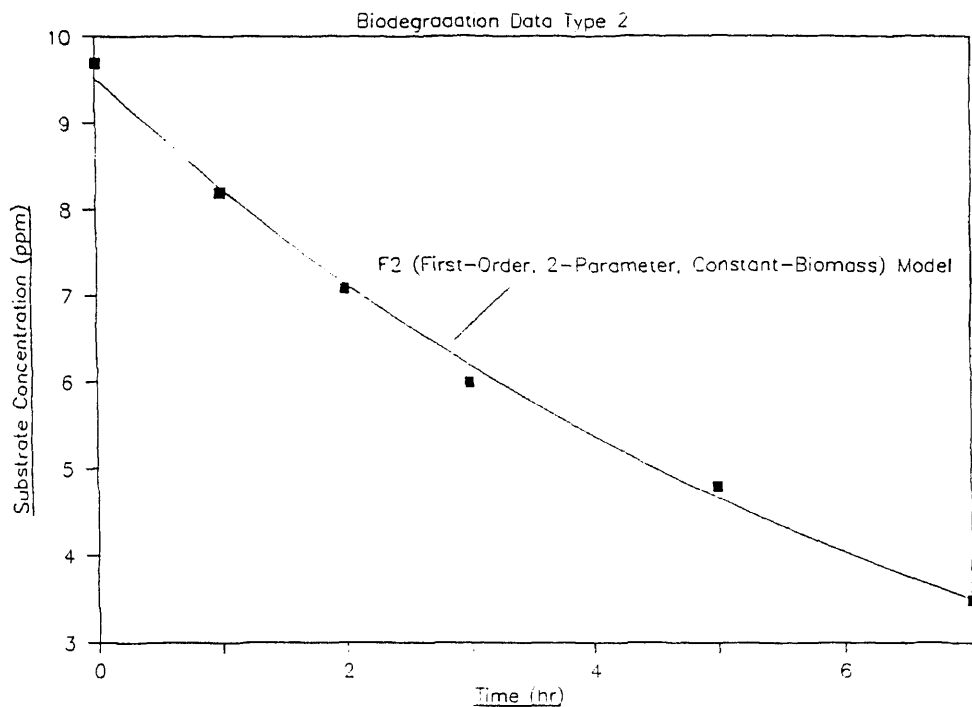
Source : Colish Thesis (data set #1) ; refer to pages E-6 & 7

Figure 14



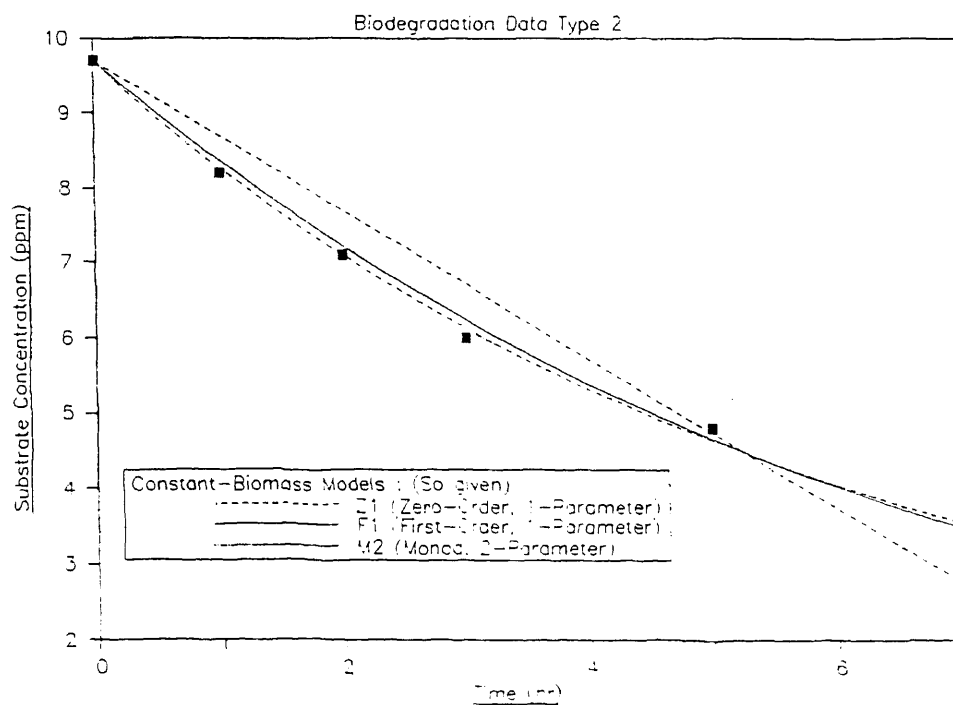
Source : Gonnabathula Thesis ; refer to data sets #1A, #2A & #6B on pages E-20, 22 & 31, respectively.

Figure 15



Source : Naik Thesis (data set #3B) ; refer to page E-65

Figure 16



Source : Naik Thesis (data set #3B) ; refer to page E-65



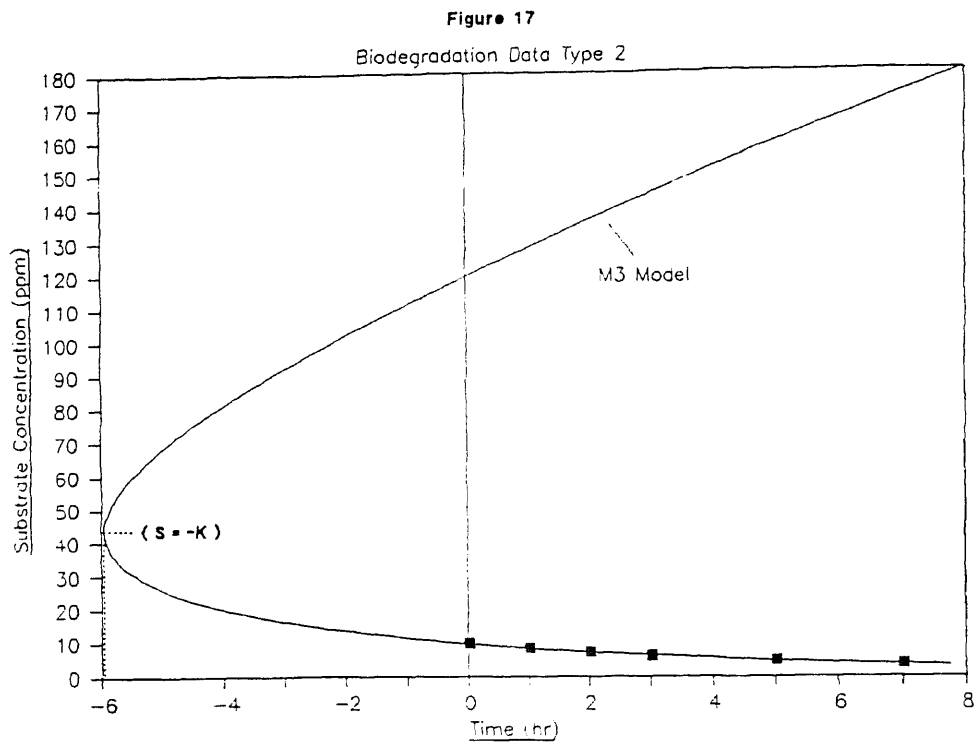
The Monod models, as before for zero-order data (i.e., data type 1), yield the statistically best results for first-order data. Whereas the Monod model (i.e.,  $-dS/dt = kS/(K+S)$ ) reduces to zero-order kinetics for high substrate concentrations (i.e.,  $S \gg K$ ), it assumes first-order kinetics at low substrate concentrations (i.e.,  $S \ll K$ ) with the resulting first-order rate constant being equal to  $k/K$ . The Monod model is statistically superior to both the zero- and first-order models in all cases because of the additional regressable parameter  $K$ , which gives it greater flexibility in fitting any set of experimental data.

While the Monod model is inherently better at minimizing  $\Sigma(t-t_{calc})^2$ , it does not necessarily mean that it better represents reality. The Monod model may incorrectly alter the curvature in otherwise purely first-order data (or similarly for zero-order data) by overfitting; an extreme example of overfitting is the manner in which an  $n$ th-order polynomial will fit a smooth curve through every data point even though the actual curve would not because of some degree of inherent experimental error in the data. This effect, however, is typically so slight for the case of the Monod model that it is negligible, especially for data with minimal experimental error. The more notable problem with the Monod model for first-order data is the possibility of regression yielding negative values for both kinetic rate constants  $k$  and  $K$  (refer to page E-65). Linear regression will yield negative values for the Monod models for all cases where  $S$  is observed

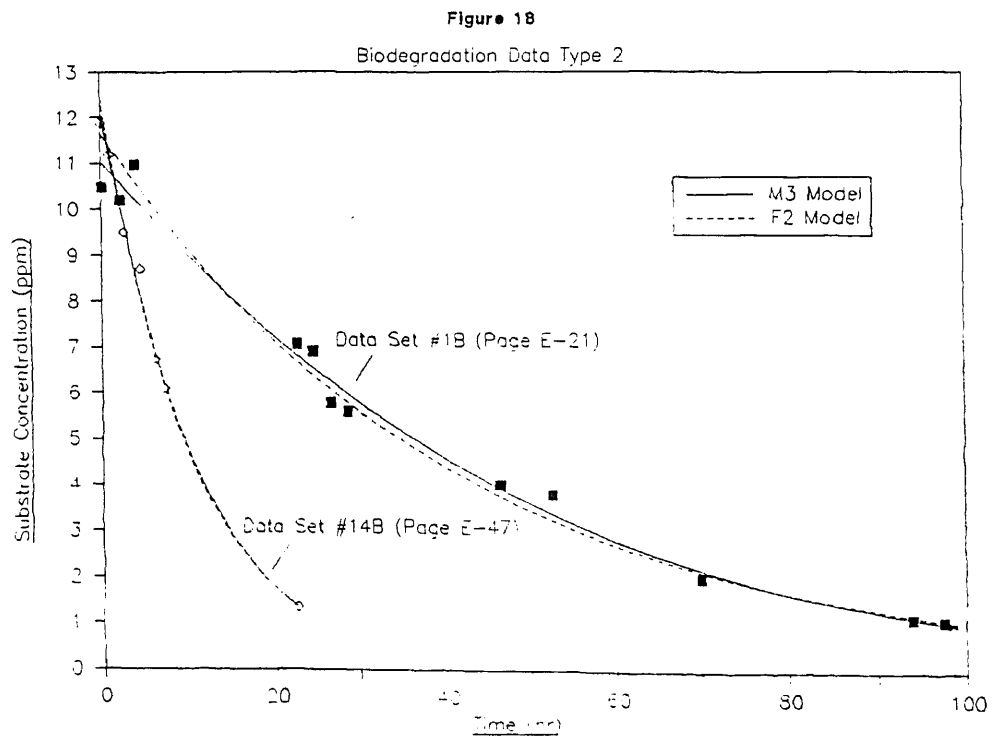
to drop at a greater than first-order rate, and positive values when the drop is less than or equal to first-order. For any experimentally measured first-order data, there is an approximately equal probability of regression yielding either both negative rate constants or both positive, depending on whether the scatter in the data can be interpreted as making the overall set greater than or less than first order, respectively.

Negative rate constants have no physical meaning and consequently invalidate any theoretical basis in the Monod models. Furthermore, practical use of the model is limited by the fact that  $-dS/dt$  becomes indeterminate when  $S$  equals the absolute value of  $K$ . This problem is displayed graphically in Figure 17 which shows an expanded version of the M3 curve. This regressed curve doubles back on itself at a value of  $S$  equal to the absolute value of  $K$ . A comparison of Figure 17 ( $k$  and  $K$  both negative) with Figure 7 ( $k$  positive and  $K$  negative) shows them to be, in effect, mirror images of one another relative to the ordinate.

The first-order models are statistically only slightly inferior to the corresponding Monod models for the data set on page E-65, while Figures 15 and 16 show both F1 and F2 to well represent the data. The first-order models are technically sound in that they always yield positive rate constants for type 2 data and, as such, are generally preferred over the Monod models for this application.



Source : Naik Thesis (data set #3B) ; refer to page E-65



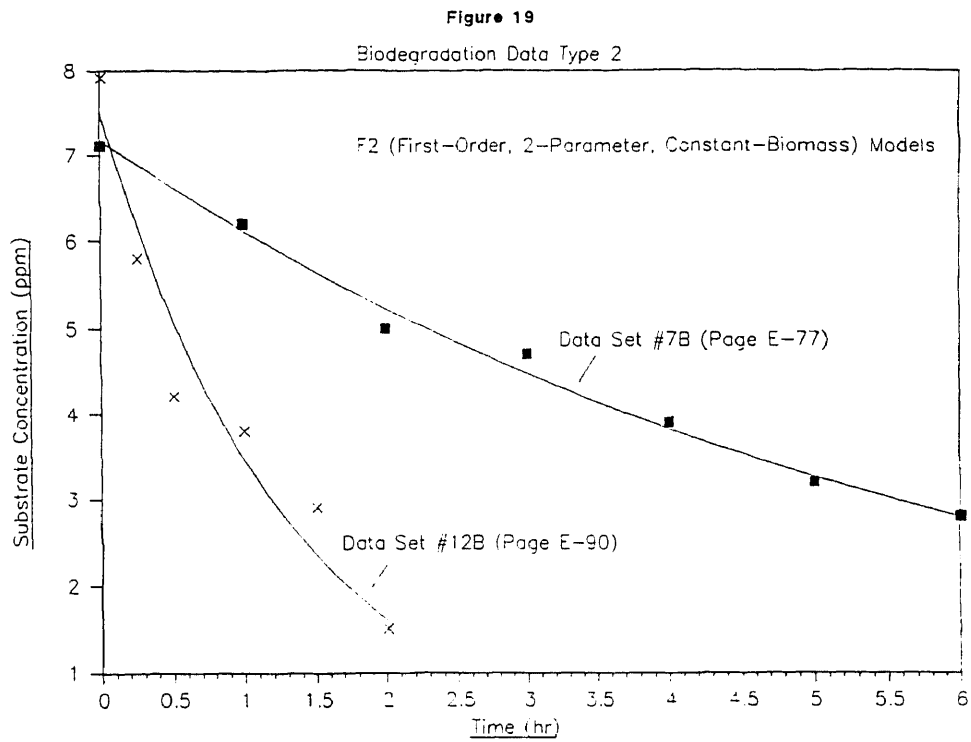
Source : Gannabathula Thesis (data sets #1B & 14B) ; refer to pages E-21 & 47

F2 is preferred to F1 because of its inherent ability to result in statistically better fits.

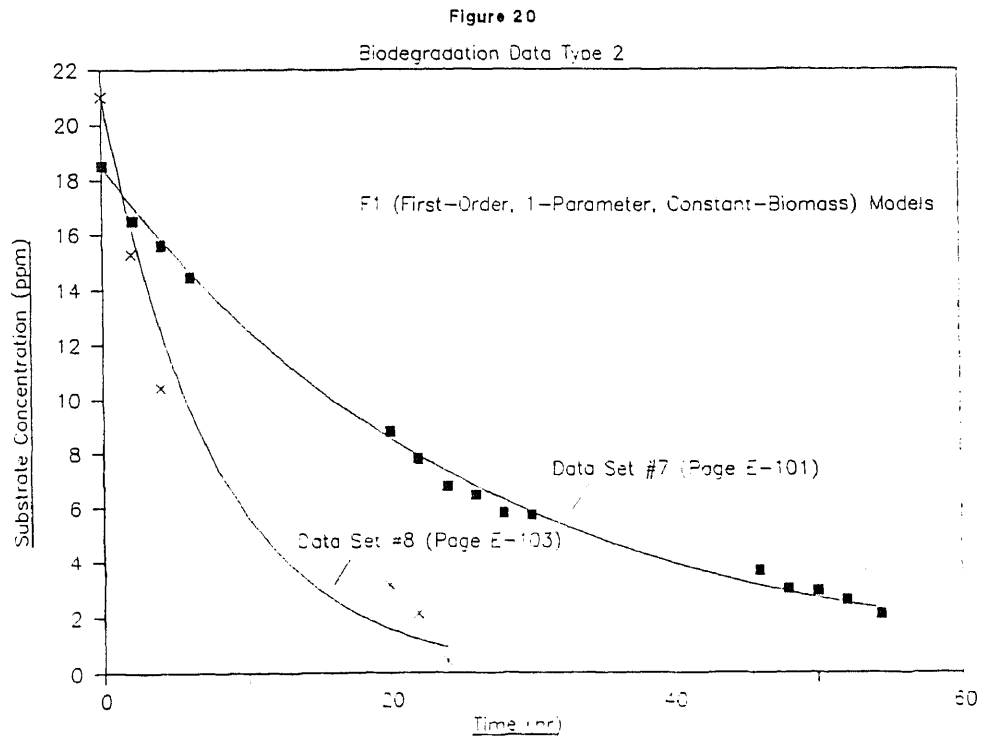
The zero-order, constant-biomass models are inappropriate for the above data because of their inherent inability to represent the necessary curvature which, in turn, accounts for them being the statistically worst of the group studied. Their inadequacy for modelling type 2 data is further magnified when extrapolating below the range of  $S$  used to regress them.

Figure 18 presents two more data sets of the second biodegradation data type with the regressed M3 and F2 curves shown for both cases. Both sets are for systems with low values of  $S/B$  and they exhibit a slightly increased amount of scatter vs. the set shown in Figure 15. Statistically and visually the models from all three sets perform comparably. The only notable difference between these two sets and the previous one is that the scatter in the former two is such that the Monod models interpret the biodegradation rates as being slightly less than first-order, thereby resulting in the regression of positive values of  $k$  and  $K$  for both data sets.

Figure 19 graphically presents the regressed F2 curves for the data sets shown on pages E-77 and E-90. Both of these sets are for the same substrate (i.e., nitrobenzene) but different activated sludge systems. The latter system uses a phenol-acclimated sludge (vs.



Source : Naik Thesis (data sets #7B & #12B) ; refer to pages E-77 & 90



Source : Pak Thesis (data sets #7 & #8) ; refer to pages E-101 & 103

an unacclimated sludge in the former) which accounts for its increased biodegradation activity as reflected in the notably higher first-order rate constants (i.e.,  $k(F2)$  of 0.77/hr vs. 0.16/hr). Both of these sets exhibit increased scatter as compared to the previous three sets shown, resulting in statistically less significant differences between all of the models studied (compare  $\Sigma(t-t_{calc})^2$  on pages E-77 and E-90). It should be noted that, for the data set shown on page E-90, M3 regresses positive rate constants while M2 yields negative values. This is the combined result of the specific scatter in the data set and the relaxed restriction of  $S_0=S(t=0)$  for the M3 model. The M3 model has no real advantage over the M2 model in terms of regressing positive rate constants. An equal probability exists for the above situation to be reversed (i.e., positive  $k(M2)$  and  $K(M2)$  and negative  $k(M3)$  and  $K(M3)$ ) depending primarily on the specific orientation of the data scatter.

Figure 20 presents two different sets of data for the same substrate/culture system (i.e., 2-chlorophenol/unacclimated sludge) along with the corresponding regressed F1 curves. The regression analysis results for the two sets are presented on pages E-101 and E-103. Whereas Pak designated both activated sludges as "unacclimated", the data set shown on page E-103 actually used the sludge from the set shown on page E-101. As a result of the sludge's previous exposure to the substrate, it had become partially acclimated accounting for the observed ca. three-fold increase in biodegradation rate (i.e.,  $k(F1)$  of

0.13/hr vs. 0.038/hr). This example illustrates the importance of properly characterizing and quantifying the biocatalyst system in order to obtain usable kinetic data and, hence, applicable models.

The data set from page E-101 (shown graphically in Figure 20) was accompanied by biomass measurements facilitating the regression analysis shown on page E-102. The variable-biomass models yielded results comparable to the corresponding lower-parameter, constant-biomass models for the following reasons: (1) no variable-biomass effect was evident in the raw  $S$  vs.  $t$  data, and (2) the measured value of  $B$  represented the "total" microbial mass, and not the "viable" biomass, which resulted in  $B$  being so high relative to  $S$  that it was effectively constant over the range considered (i.e., based on the values of  $B_0$  and  $Y_c$ ,  $B$  increases by only 11% during the experiment). It should be noted that the values of  $B_0$  and  $Y_c$  used are very suspect. A value of  $Y_c$  greater than 1 can only be explained by either unaccounted-for substrate utilization or inaccurate  $B$  measurements. The latter is more than likely the case in this situation.

The regression results on pages E-101 and E-102 show that M2, M3 and MV all yield negative values for both  $k$  (or  $k_0$ ) and  $K$  because of an apparent greater-than-first-order drop. In general, MV will yield negative values for  $k$  and  $K$  in the same cases as the M2 model, providing  $Y_c$  is positive. If  $Y_c$  were negative, however, MV could regress positive values of both  $k$  and  $K$  in situations where the

constant-biomass versions do not. The effect of the negative  $Y_c$  is to allow MV to fit a greater-than-first-order drop with positive rate constants; the more negative  $Y_c$  is, the higher the drop that MV can fit with positive rate constants. The problem with this, however, is that a negative value for the substrate-specific parameter,  $Y_c$ , is theoretically invalid. As substrate is consumed, a portion of the substrate is utilized by the "viable" biomass for growth, thereby always resulting in positive values of  $Y_c$ .

In addition to the 7 data sets discussed thus far in this subsection, 2 more of the 124 mixed-culture data sets evaluated in this thesis have been classified as type 2 (refer to Figure 21). Both of these sets were extracted from the open literature. Neither author reported analytical accuracy (Lyons did, however, indicate reproducibility by performing measurements in triplicate and reporting mean values of  $S$  with calculated standard deviations), adequate biomass data (Lyons reported none while Wong's data was insufficient for determining  $B_0$  and  $Y_c$  for variable-biomass modelling purposes), nor performed any kinetic analyses. Both studies were more interested in qualitative assessment and relative rates of biodegradation than generating data useful for engineering design purposes. Lyons' data set showed little scatter and yielded positive values of  $k$  and  $K$  for both M2 and M3 while Wong's data set exhibited significant scatter and yielded negative values of  $k$  and  $K$  for both M2 and M3. The scarcity of data points in the latter case, along with the apparent high degree of experimental



Figure 21

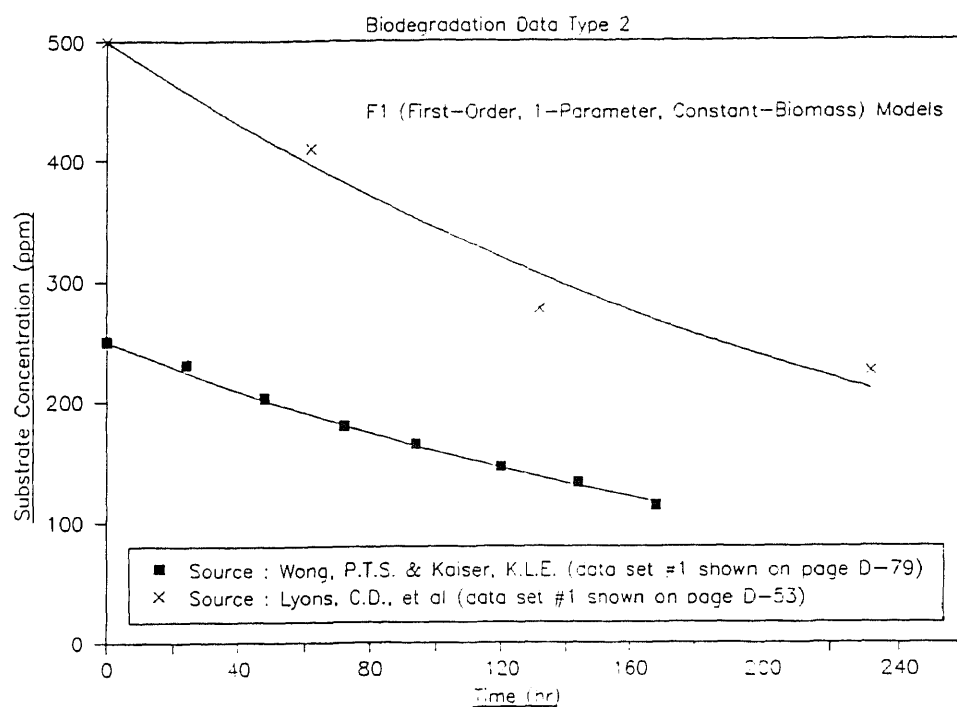
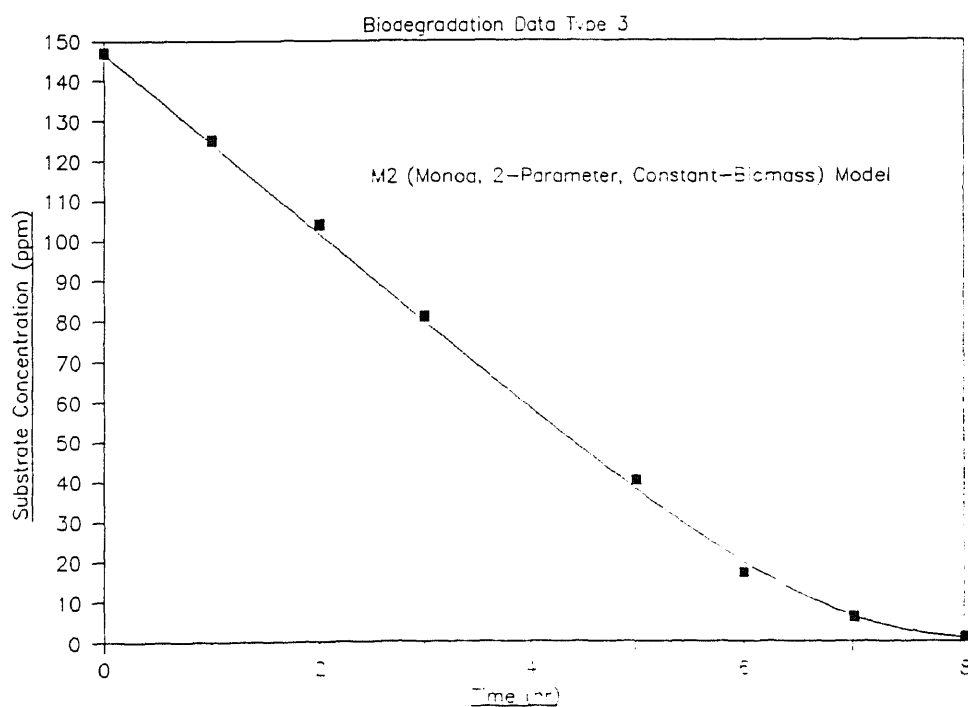


Figure 22



uncertainty makes model differentiation extremely difficult.

In order for the data shown in Figure 21 to have been of practical use to other scientists and engineers, the authors should have done the following: (1) reported the analytical accuracy of S values, (2) provided accurate measurement of "viable" biomass concentration, as well as a taxonomic definition or history of the culture, and (3) measured more than four S vs t data points. Wong did, however, to his credit eliminate abiotic effects (i.e., adsorption and stripping) from the S vs t data.

#### 6.1.3 Data Type 3 (Monod, Constant Biomass)

Of the 124 mixed-culture, batch-reactor, raw aerobic biodegradation data sets evaluated in this thesis, 24 were categorized as type 3 or the Monod, constant-biomass type (refer to Figure 22). These sets are intermediate in order between zero and one. Some sets are mostly zero-order with a switch to the first-order regime at lower values of S, while others are mostly first-order. Data sets spanning the entire range of zero- to first-order are present. Both the zero- and first-order models are inappropriate for representing data of this type. The behavior of the zero-order models are analogous to that described in Section 6.1.2 for the fitting of first-order data, although the inadequacies are not as extreme, especially for the cases where the data sets are mostly in the zero-order realm. The same goes for the behavior of the first-order models being analogous to that described in

Section 6.1.1 in the fitting of zero-order data, with the inadequacies becoming less evident as the reaction order approaches one.

Figure 22 shows the data set from page D-69 to be well represented by the M2 model. The data has little scatter accounting for M3 being statistically only marginally better than M2. The other models are significantly worse. The data is basically zero-order down to an S value of ca. 40 ppm, at which point the transition to first order begins to take place. The transition from the zero- to the first-order regimes varies from experiment to experiment depending upon: (1) substrate type, (2) biomass type (i.e., concentration and composition), and (3) a myriad of other environmental conditions such as temperature and pH. It is apparent based on the above that prediction of biodegradation data type from the order of magnitude of S alone is not feasible.

The data set shown in Figure 22 was extracted from the open literature. Saeger and Tucker did not report analytical accuracy, measure biomass data, nor perform any kinetic analyses. Whereas non-biodegradation mechanisms (i.e., chemical oxidation and volatilization) were determined to be negligible, and whereas very little data scatter is apparent, the data presented in Figure 22 are of little use for design purposes without a quantitative measure of the "viable" biomass concentration.

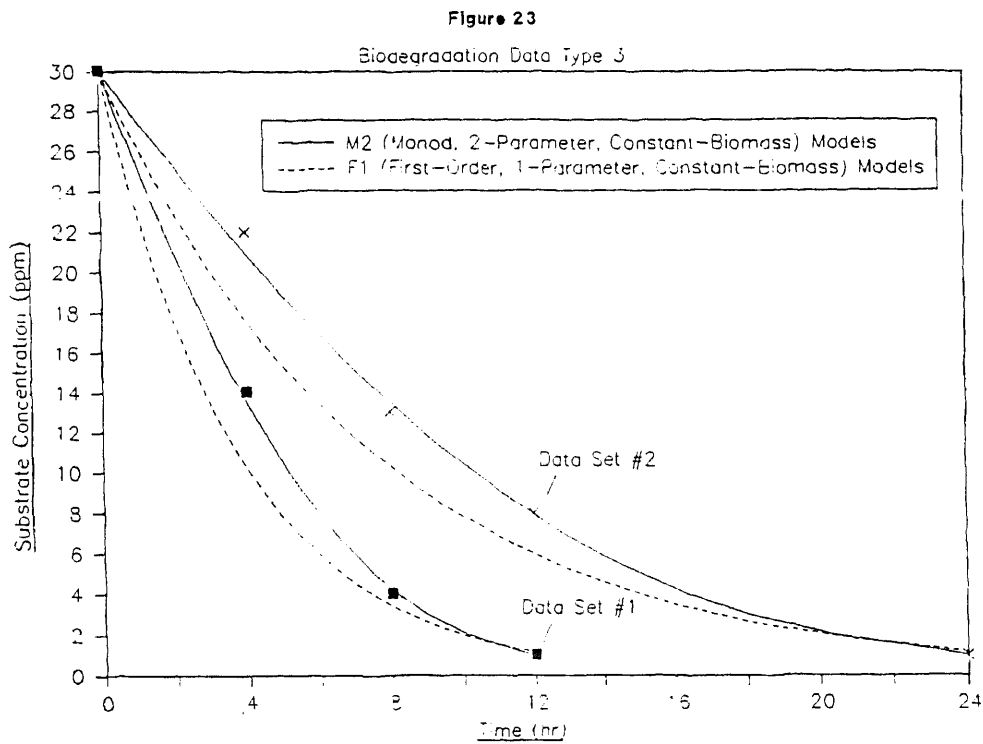
Figure 23 presents two data sets of biodegradation type 3, both of which were experimentally measured by Sayler, et al. In the article, the authors stated that the experiments were not well designed to determine reaction order. The data sets were said to be suggestive of first order, although the possibility of fractional-order kinetics was not ruled out. Even after the authors' expression of their awareness of their uncertainty with respect to reaction order, they incorrectly modelled and presented the kinetics as first-order. Figure 23 graphically shows (as the tabulations on pages D-70 and D-71 statistically do) that the data sets are clearly less than first order. As a side note, the first-order rate constants presented by Sayler, et al., are in agreement with those determined in this thesis (refer to Table 3 below).

Table 3

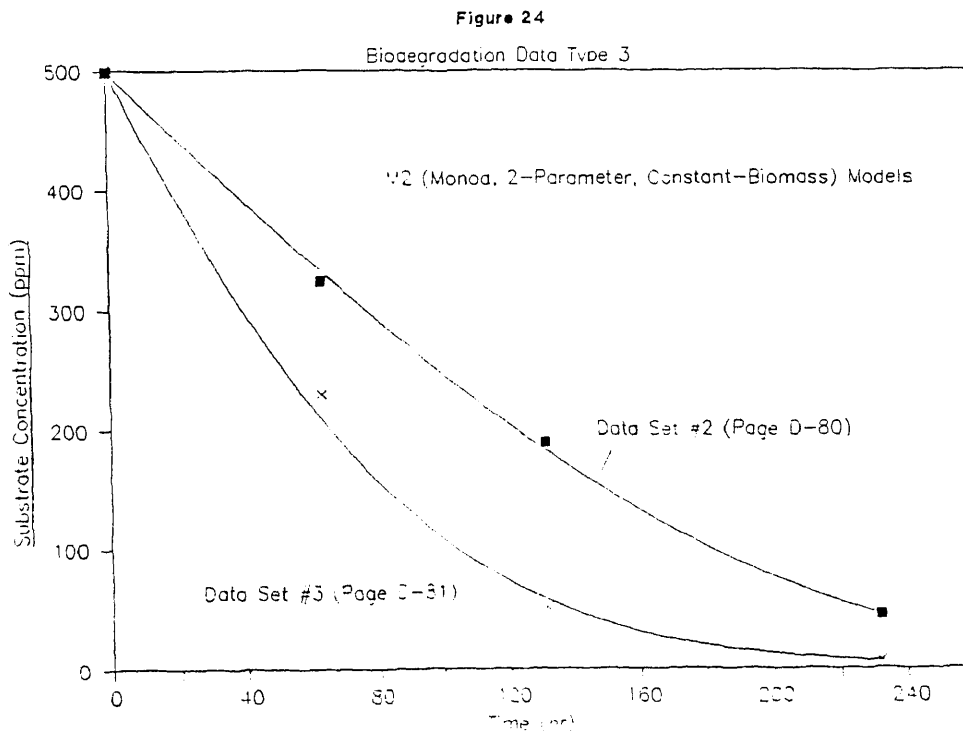
Regressed First-Order Rate Constants for Data Sets #1 and #2

on Pages D-70 and 71 (Source: Sayler, et al.)

| <u>Data Set</u> | <u>Regressed Literature<br/>Value of <math>k</math> (1/hr)</u> | <u>Regressed Thesis Value of <math>k</math> (1/hr)</u> |                           |
|-----------------|--|--|---------------------------|
|                 |  | <u><math>k(F1)</math></u>                              | <u><math>k(F2)</math></u> |
| #1              | 0.28   | 0.270  | 0.291                     |
| #2              | 0.14   | 0.134  | 0.147                     |



Source : Saylor, G.S., et al (data sets #1 & #2 shown on pages D-70 & 71)



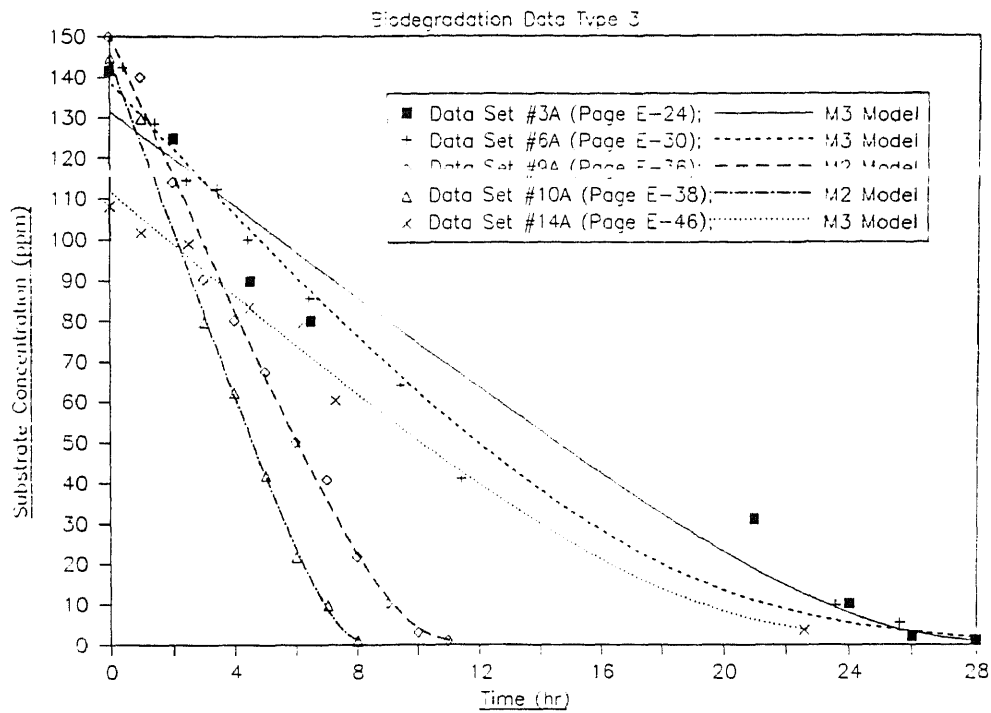
Source : Wong, P.T.S. & Kaiser, H.L.E. (data sets #2 & #3 on pages D-80 & 81)

While the data sets presented in Figure 23 have minimal scatter and are well represented by the Monod models, they are of no practical use for design purposes due to the lack of qualitative and quantitative information about the activated sludge system. No difference between the sludge used in the two data sets was indicated by the authors, yet a two-fold difference in biodegradation rate was observed for the two purportedly identical systems and conditions.

Figure 24 presents two more data sets of biodegradation type 3, both of which were experimentally measured by Wong and Kaiser. These two sets were extracted from the same article as that data set shown in Figure 21 and the same general comments made on pages 48 and 50 for that set are applicable here except for the fact that it was interpreted as type 2 data (note: all three sets are for different substrates and, as a result, have different biodegradation rates).

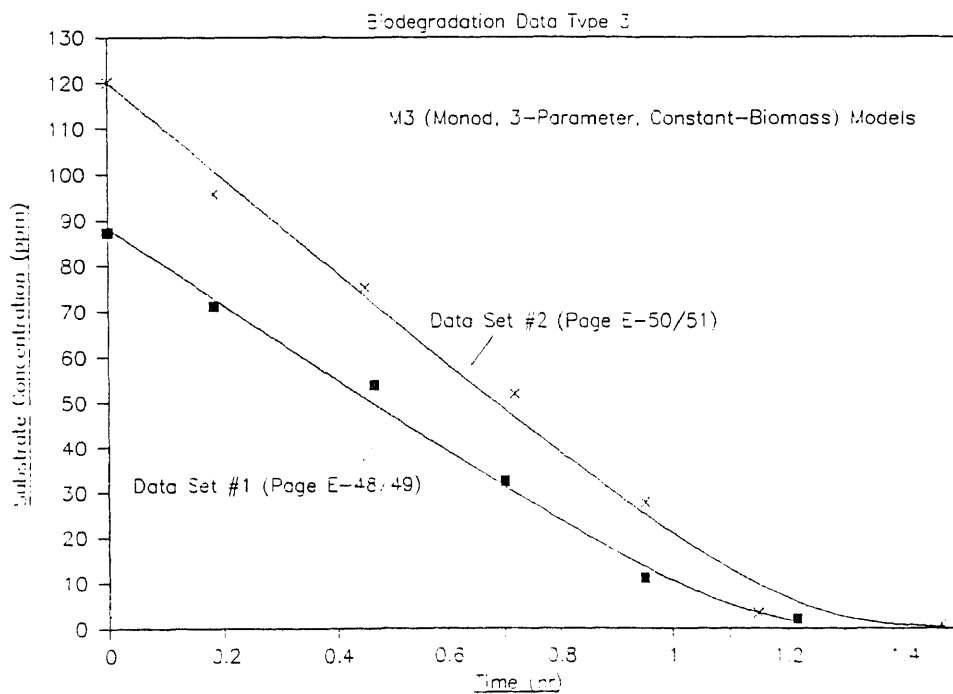
Figure 25 graphically presents five data sets from Gonnabathula's thesis which are for the same substrate (i.e., phenol) and are all of the same biodegradation type (i.e., type 3). All five sets were measured under virtually identical experimental conditions (e.g.,  $\text{NH}_3$  content, MLSS level and temperature) except for co-substrate type. Table 4 summarizes below the Monod rate constants for each set and specifies the co-substrate used in each case. Significant variability between the results for the same substrate and conditions,

Figure 25



Source : Gonnabathula Thesis

Figure 26



Source : McMullen Thesis (data sets #1 & #2 on pages E-48/49 & 50/51)

even for the cases with the same co-substrate, is apparent. In each of the five sets shown in Figure 25, not only does the rate of the zero-order drop vary (as reflected in the  $k(M3)$  values varying ca. 400% from 6.18 to 23.29), but so does the point at which transition to first-order kinetics begins (as reflected in the  $K(M3)$  values varying ca. 400% from 8.50 to 37.12). These results differ from one another because of subtle differences in the activated sludges which were not sufficiently represented by crude MLSS measurements. Knowledge of the biocatalyst amount, type and history is critical to the measurement and utilization of biodegradation data.

Table 4

Regressed M3 Model Rate Constants for Phenol as Substrate  
in Activated Sludge (Data Source: Gonnabathula Thesis)

| <u>Data Set</u> | <u>Co-Substrate</u> | <u><math>k(M3)</math>, ppm/hr</u> | <u><math>K(M3)</math>, ppm</u> |
|-----------------|---------------------|-----------------------------------|--------------------------------|
| #3A             | 2,6-dichlorophenol  | 6.18                              | 8.76                           |
| #6A             | 2-chlorophenol      | 10.61                             | 37.12                          |
| #9A             | 2-chlorophenol      | 19.07                             | 11.93                          |
| #10A            | 2-chlorophenol      | 23.29                             | 8.50                           |
| #14A            | Nitrobenzene        | 7.59                              | 18.36                          |

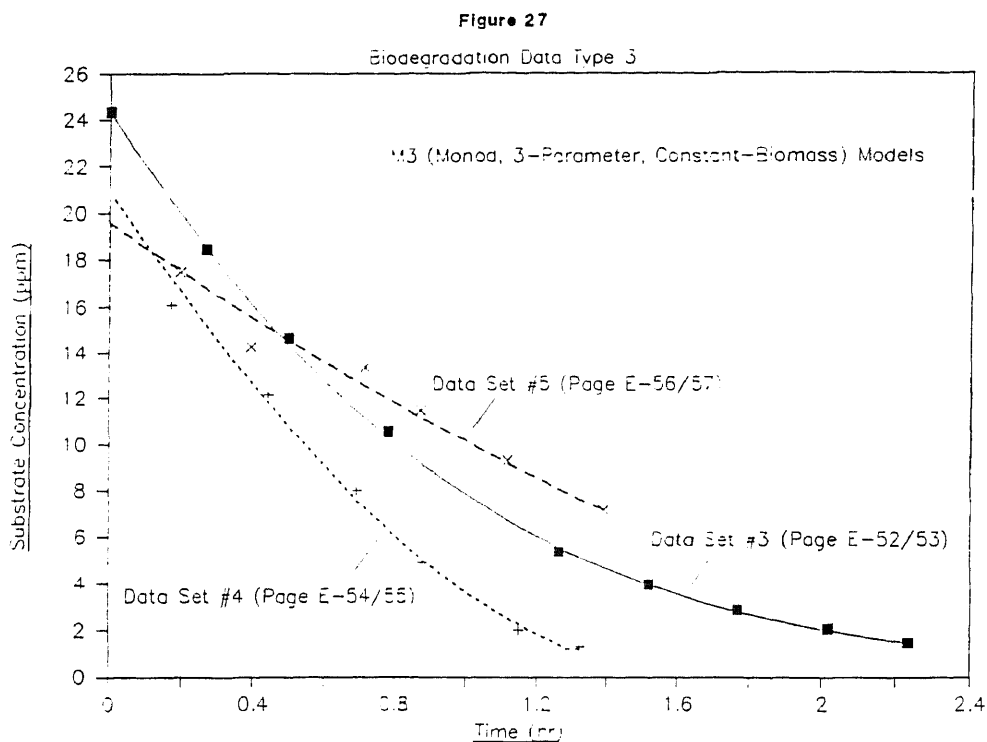


Figure 26 presents two other data sets of biodegradation type 3 for the substrate phenol (this time as the sole carbon source) in activated sludge. The degradation is much more rapid in these two sets as compared to those shown in Figure 25, which may either be due to inhibitory effects of the co-substrates used by Gonnabathula, or just to inherent differences in the activated sludges. It should be noted that MLSS measurements by McMullen were ca. 50% higher for data set #1 vs. data set #2 (refer to pages E-49 and E-51, respectively), yet the latter set exhibited more rapid biodegradation. The reason for this is that the sludge from the first set was used as inoculum for the second; partial acclimation had occurred with growth of the substrate-specific bacteria while the bulk of the biomass (being non-viable) decreased, resulting in lower MLSS values. This further exemplifies the inadequacy of MLSS measurement as a gauge of biocatalyst activity.

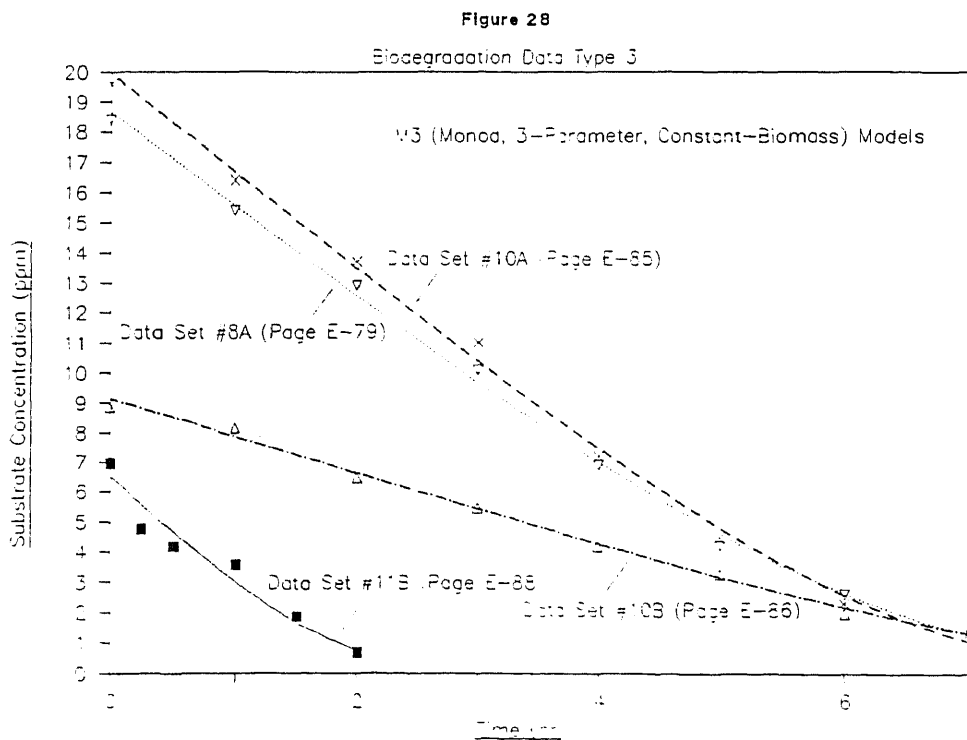
Pages E-49 and E-51 summarize the regression results for variable-biomass models for the two data sets shown in Figure 26. The variable-biomass models are no better than the constant-biomass versions for this data type because no variable-biomass effects are evident; the variable-biomass effects present in the data sets discussed in this subsection are negligible relative to the experimental uncertainties in the data. Furthermore, the values of  $B_0$  and  $Y_c$  are based on crude MLSS measurements causing the variable-biomass models to yield results of questionable validity. Page E-49 shows the substrate-specific parameter  $Y_c$  to be -0.617, which is not theoretically valid.

Gonnabathula also provided MLSS measurements for all of his biodegradation data sets as McMullen did. Variable-biomass models were not evaluated in the former case, however, because of the additional complication of co-substrates being present.  $Y_c$  is a substrate-specific parameter and no reliable method is available to calculate it from bulk mixture measurements.  $Y_c$  can only be accurately determined for single-substrate systems. Application of  $Y_c$  values determined in this manner to multiple substrate systems may not necessarily be valid due to potential interactive effects.

Figure 27 graphically presents three data sets for 2-chlorophenol as sole substrate in activated sludge, as measured by McMullen under virtually the same conditions (refer to pages E-52 through E-57). Table 5 below again shows the significant variation, in terms of the regressed rate constants, between repeated experiments run under presumed identical conditions. Better definition and control of the reaction system in terms of key parameters (e.g., biomass type/amount, nutrients, temperature, agitation, etc.) are required to obtain reliable data and models. Based on the observed trend in the tabulated data and the fact that the inoculum to each set is the activated sludge from the previous set, it appears that the viable biomass concentration is dropping (along with the total biomass concentration, as indicated by the calculated negative values of  $Y_c$ ), possibly due to some inhibitory or toxic effect associated with utilization of the substrate.



Source : McMullen Thesis (data sets #3, #4 & #5 on pages E-52/53, 54/55 & 56/57)



Source : Naik Thesis (data sets #8A, #10A, #10B & #11B on pages E-79, 85, 86 & 88)

Table 5

Regressed M3 Model Rate Constants for 2-Chlorophenol as  
Substrate in Activated Sludge (Data Source: McMullen Thesis)

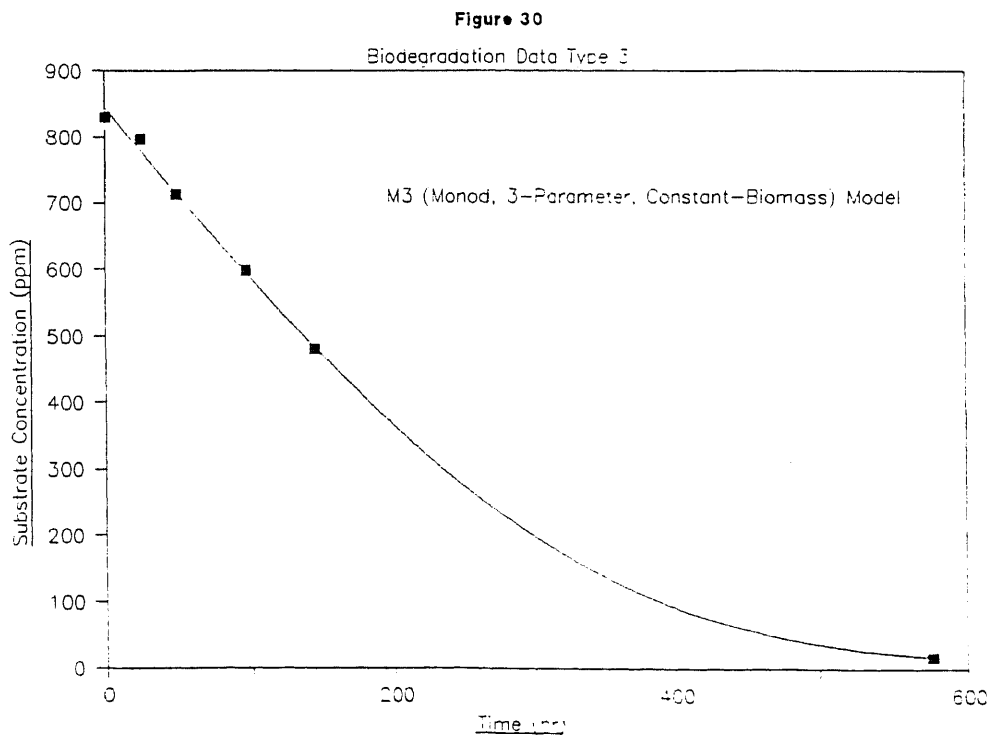
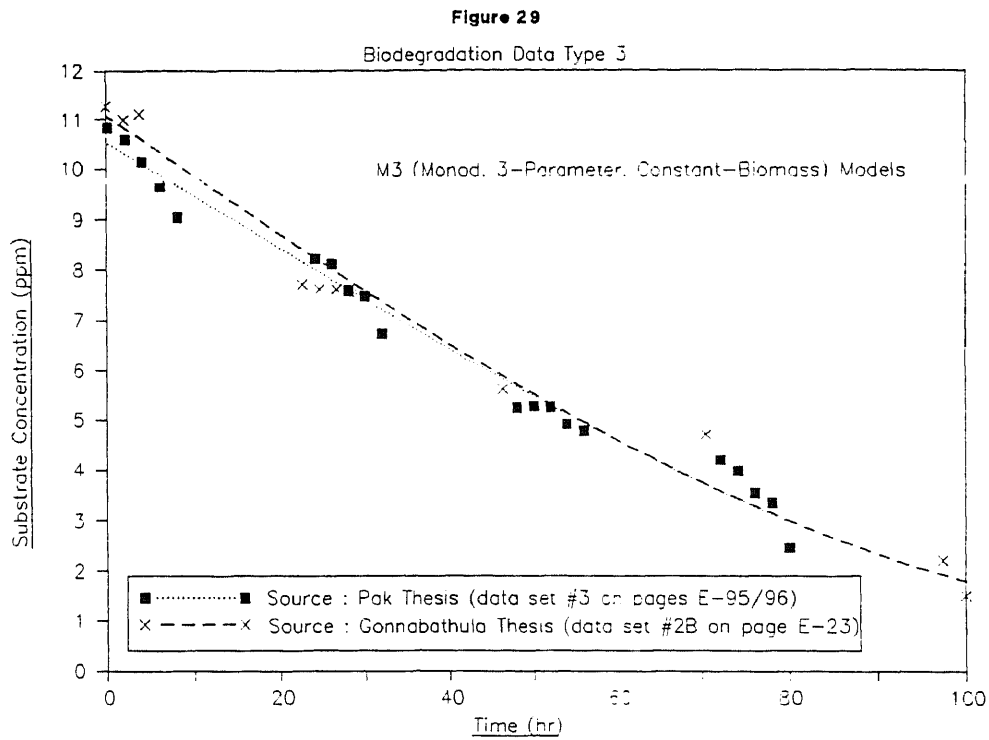
| <u>Data Set</u> | <u>k(M3), ppm/min.</u> | <u>K(M3), ppm</u> |
|-----------------|------------------------|-------------------|
| #3              | 1.14                   | 45.4              |
| #4              | 0.52                   | 9.1               |
| #5              | 0.27                   | 10.6              |

Four more data sets of biodegradation type 3 are presented in Figure 28. All four were extracted from Naik's thesis and each involved simultaneous biodegradation of two co-substrates. Variable-biomass models were not evaluated (although no improvement would be expected over the constant-biomass versions for data of type 3) because of the inability to calculate  $Y_c$  for a specific substrate from nonsubstrate-specific bacterial measurements. Data sets #8A and #10A are duplicate experiments on 2-chlorophenol substrate with apparently good reproducibility being achieved. Data sets #10B and #11B are identical experiments (for nitrobenzene substrate) except for the sludges; the former used unacclimated sludge while the latter used phenol-acclimated sludge which, in turn, accounted for the notably higher biodegradation rate.

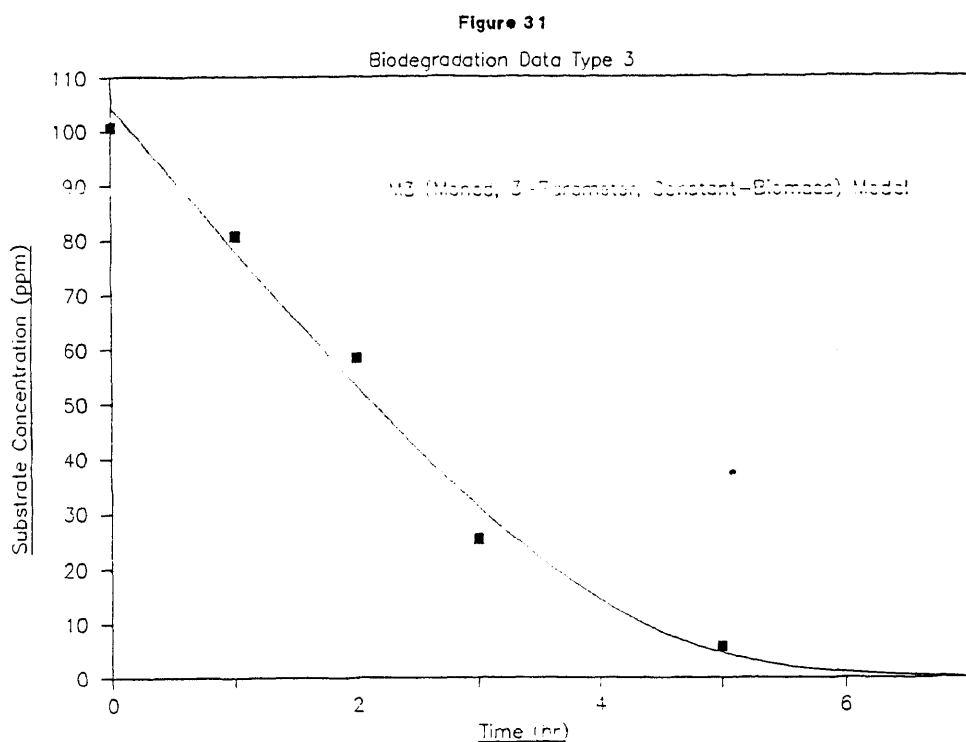
In addition to the 19 data sets discussed thus far in this subsection, Figures 29 through 32 present the 5 remaining sets studied in this thesis which were classified as biodegradation type 3.

Figure 29 shows two sets of data for the same system (i.e., 2,6-dichlorophenol in MLSS) at comparable conditions from two different sources (i.e., Pak and Gonnabathula) yielding reproducible results. While the two curves overlap reasonably well, the regressed values of  $k(M3)$  and  $K(M3)$  for the two data sets as shown on pages E-23 and E-95 still differ appreciably, specifically the  $K(M3)$  value. This demonstrates the mutual sensitivity of  $k$  and  $K$  in the Monod models to slight changes in the data as compared to the single rate-constant models. It should be noted that both of these data sets exhibit significant scatter making model differentiation difficult (refer to the  $\Sigma(t-t_{calc})^2$  values on pages E-23 and E-95). Within the accuracy of the data, the zero- and first-order models (although statistically worse) cannot be discounted with any great confidence.

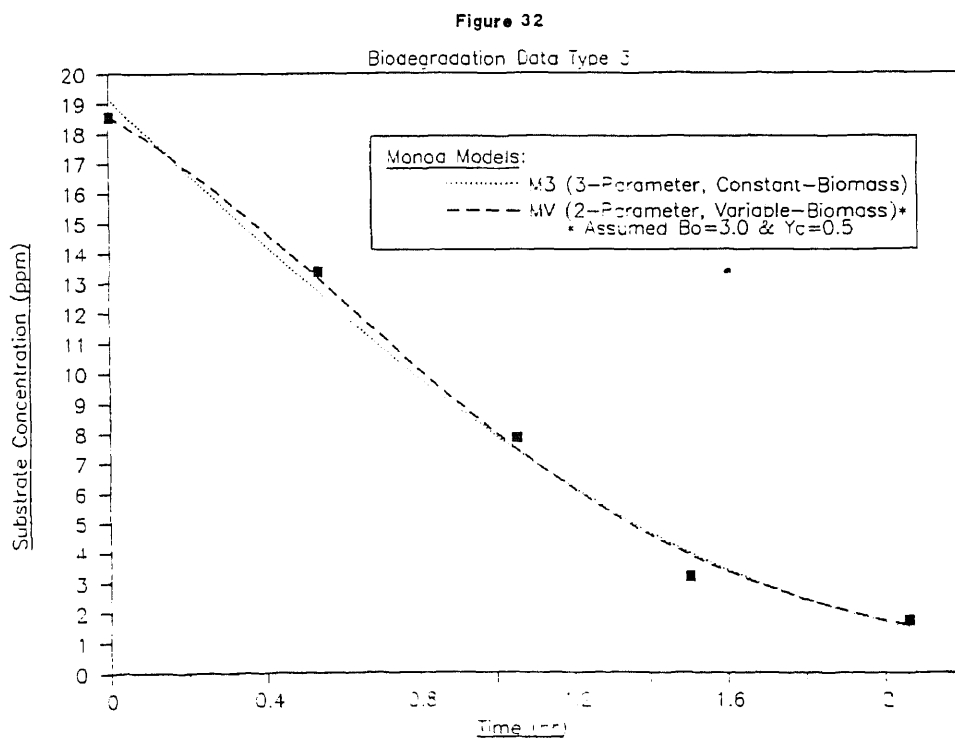
Figures 30 and 31 show two data sets that are well-represented by the M3 model. The data in Figure 30 was extracted from the open literature. As in most of the literature sources reviewed, the authors did not: (1) report analytical accuracy and (2) measure and characterize the biocatalyst. This makes the data presented of little use to others for design purposes. Taylor and Ribbons were more concerned with the study of the mechanism of metabolic breakdown of



Source : Taylor, B.F. & Ribbons, D.W. (data set #3 shown on page D-78)



Source : Naik Thesis (data set #2A shown on page E-61)



Source : Pak Thesis (data set #6 shown on page E-100)

o-phthalic acid than with providing data for design. They performed no kinetic analysis of their data.

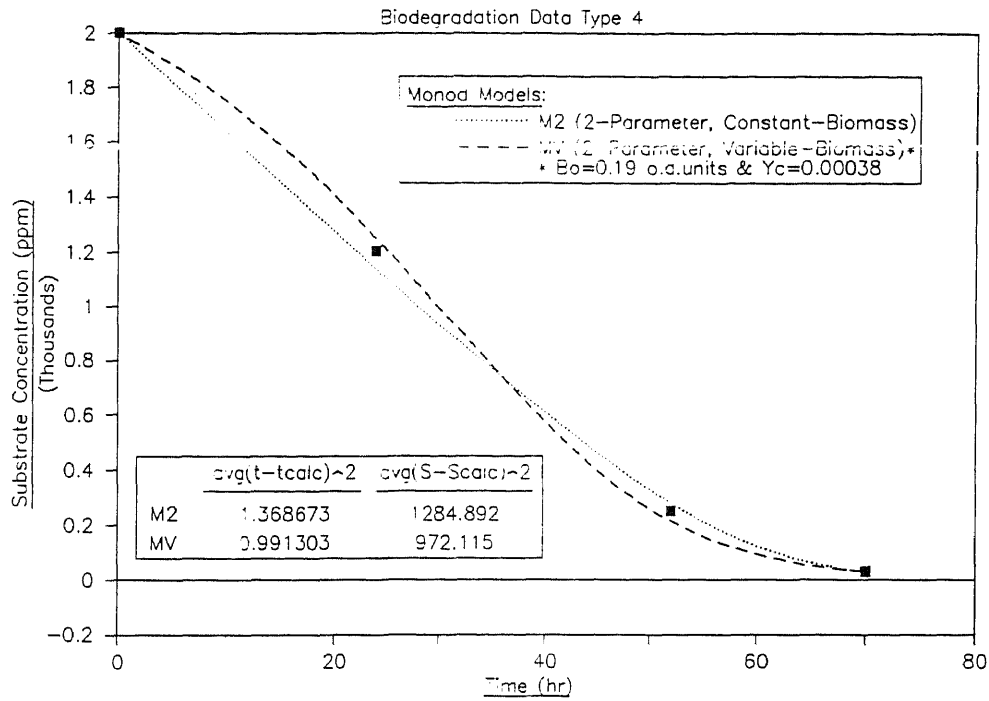
Figure 32 shows a data set which is well-represented by the M3 model to be better represented by the MV (Monod, 2-parameter, variable-biomass) model. Biomass data were not provided for this set and it is not sure whether MV is the correct interpretation of the data or whether it just happens to result in a better fit for the specific scatter present. The value of  $Y_c$  used on Figure 32 was assumed to be 0.5 (considered a typical value for  $Y_c$ ) while the value of  $B_o$  was selected so as to minimize the value of  $\Sigma(t-t_{calc})^2$  (i.e., 0.004144 vs. 0.006372 for M3). It should be noted that, while lower values of  $B_o$  (i.e.,  $<3.0$ ) resulted in even lower values of  $\Sigma(t-t_{calc})^2$ , they also resulted in the MV model regressing negative values for both  $k_o$  and  $K$ .

#### 6.1.4 Data Type 4 (Monod, Variable Biomass)

The next biodegradation data type to be discussed is the variable-biomass version of data type 3 which is well-represented by the MV (Monod, 2-parameter, variable-biomass) model as demonstrated in Figure 33 for the data set shown on page D-36. The data summary for the variable-biomass kinetic analysis of this set is not contained in the appendix, but the results are displayed graphically for each model (i.e., MV, ZV and FV) in Figures 33 and 34.

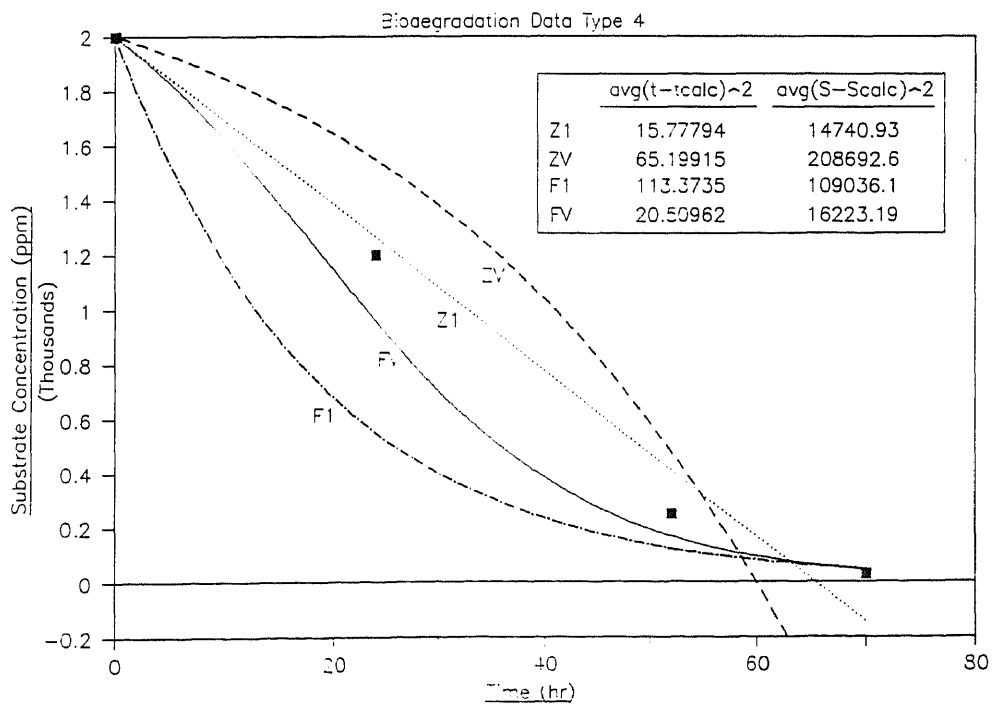


Figure 33



Source : Pyatendinov, A.N., et al (data set #3 shown on page D-36)

Figure 34



Source : Pyatendinov, A.N., et al (data set #3 shown on page D-36)

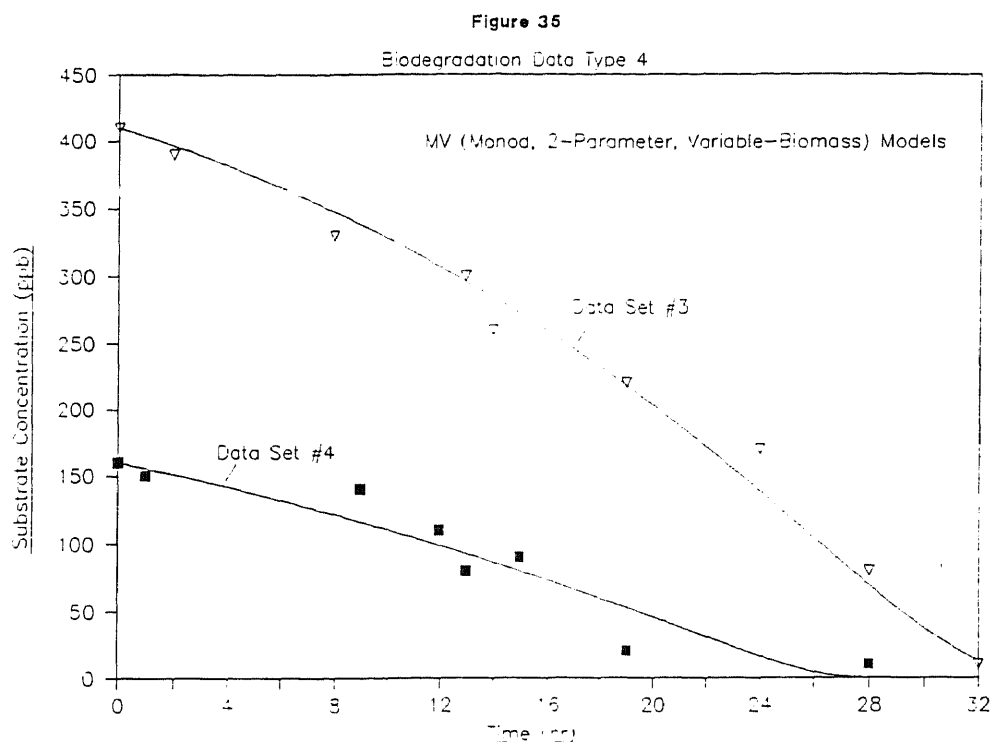
Ilyalendinov, et al, measured and presented the biomass data in optical density units as opposed to the more common concentration unit of ppm seen throughout this thesis; this accounts for the much lower numerical values of  $B_o$  and  $Y_c$ . The units of  $B_o$  and  $Y_c$  are not critical except to the extent that they are consistent with one another. The variable-biomass data presented by the authors are of better quality, even though only four data points were available, than any of the MLSS measurements discussed thus far (as demonstrated by the resulting good fit by the MV model in Figure 33). The bacterial cultures discussed previously were activated sludges, which by definition consist of a large, diverse group of bacterial species in a complex heterotrophic system. However, the culture used by Ilyalendinov, et al, consisted of a mixture of only two pure bacterial strains (i.e., B. cereus and P. aeruginosa) in a single-level trophic system. Because this mixed-culture system contained only two strains, both capable of utilizing the alpha-methylstyrene substrate (vs. an activated-sludge system where a high percentage of the bacterial strains are inactive/non-viable) in a single-trophic system (vs. a heterotrophic system where non-viable, non-bacterial microorganisms are present), this system resulted in more reliable predictions of  $B_o$  and  $Y_c$ . These

values, however, still suffer from the inaccuracies (although not nearly to as great an extent) related to the biomass measurement techniques which do not differentiate between living and dead cells. The MV model would have resulted in a better fit if a lesser variable-biomass effect had been predicted by  $B_0$  and  $Y_c$  (i.e., if  $B_0$  were higher or  $Y_c$  were lower, or a combination of both). The accuracy of  $Y_c$  used here is more suspect than  $B_0$  based on the fact that  $Y_c$  varied significantly (rather than remained constant as is a basic presumption of the variable-biomass models evaluated in this thesis) over the range of  $S$  covered. Variation of  $Y_c$  with conversion has been noted elsewhere in the literature by Pirt<sup>3</sup> and Yang and Humphrey.<sup>4</sup>  $Y_c$  varied here due to utilization of the substrate having encompassed the pre-exponential and declining-growth phases, and not just the exponential growth phase over which  $Y_c$  should remain virtually constant.

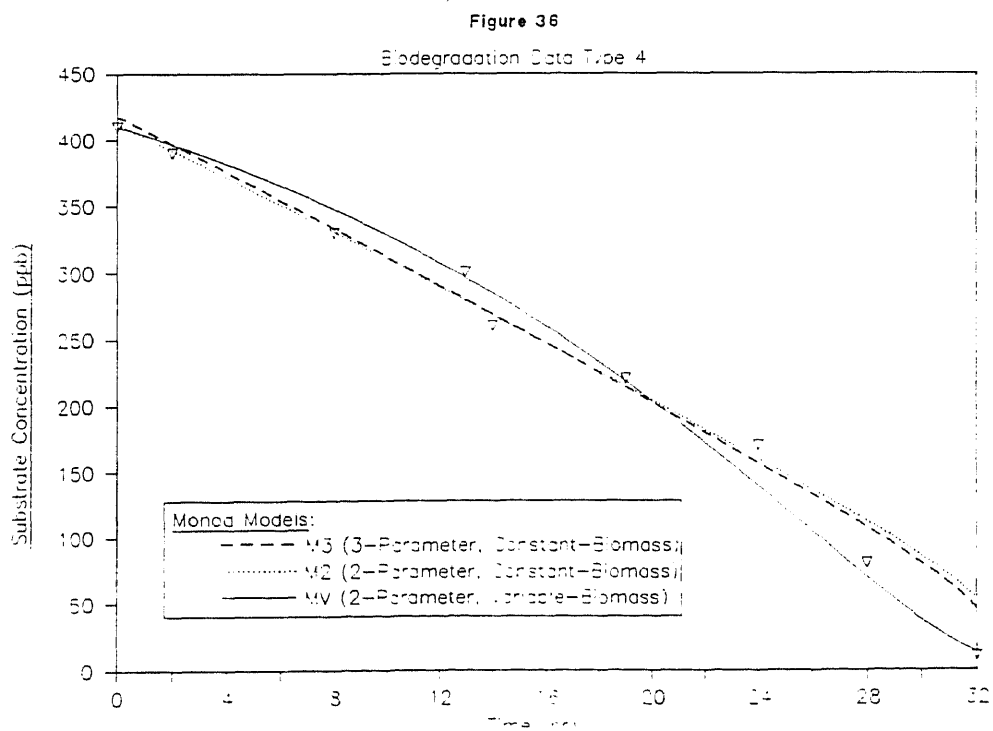
Figure 33 shows MV to be statistically and visually the best of the models evaluated. The constant-biomass Monod models, however, are not unreasonable, even though  $B$  increases five-fold over the range of  $S$  covered. Considering that there are only four data points and that the authors did not report analytical accuracy (nor did they perform any kinetic analysis), M3 and M2 cannot be discounted with complete confidence as incorrect representations of the system.

Figure 34 shows the lower-parameter, constant-biomass versions of the zero- and first-order models along with the corresponding variable-biomass versions. None of the models are good for the data set shown. Because of the nature of Monod kinetics spanning the range from zero to first order, there will be instances where the type 4 data will be mostly zero order and, hence, will be reasonably well represented by ZV; analogously, the type 4 data may on occasion be mostly first order and, hence, will be well represented by FV. The extent to which the constant-biomass models are reasonable for such data depends on the extent to which B varies. The general characteristics of FV and ZV for typical type 4 data are visually demonstrated in Figure 34. A more detailed discussion of the characteristics of each of the variable-biomass models and their sensitivity to the parameters  $B_0$  and  $Y_c$  will be provided later in this section.

Figure 35 provides two data sets of type 4 for pentachlorophenol substrate in MLSS for two different values of  $S_0$ . The values for  $k_0$  and  $K$  on pages D-46 and D-48 for the two sets are quite different. This difference in biodegradation rate is attributed by Klecka and Maier to substrate inhibition. They took this into account when they modelled the data by using the Haldane modification of the Monod equation:



Source: Klecka, G.M. & Maier, W.J. (data sets #3 & #4 on pages D-45 thru 48)



Source: Klecka, G.M. & Maier, W.J. (data set #3 on pages D-45 & D-46)

$$-\frac{dS}{dt} = \frac{\mu B}{Y_c} \left( \frac{S}{K+S+S^2/K_I} \right) \quad ; (1)$$

where,

$$k = \frac{\mu B}{Y_c} = k_o B$$

$\mu$  = maximum bacterial growth rate

$S^2/K_I$  = substrate inhibition term

$K_I$  = substrate inhibition constant

They also incorporated an endogenous decay coefficient ( $k_D$ ) within the biomass equation:

$$\frac{dB}{dt} = \frac{\mu B}{Y_c} \left( \frac{S}{K+S+S^2/K_I} \right) - k_D B \quad ; (2)$$

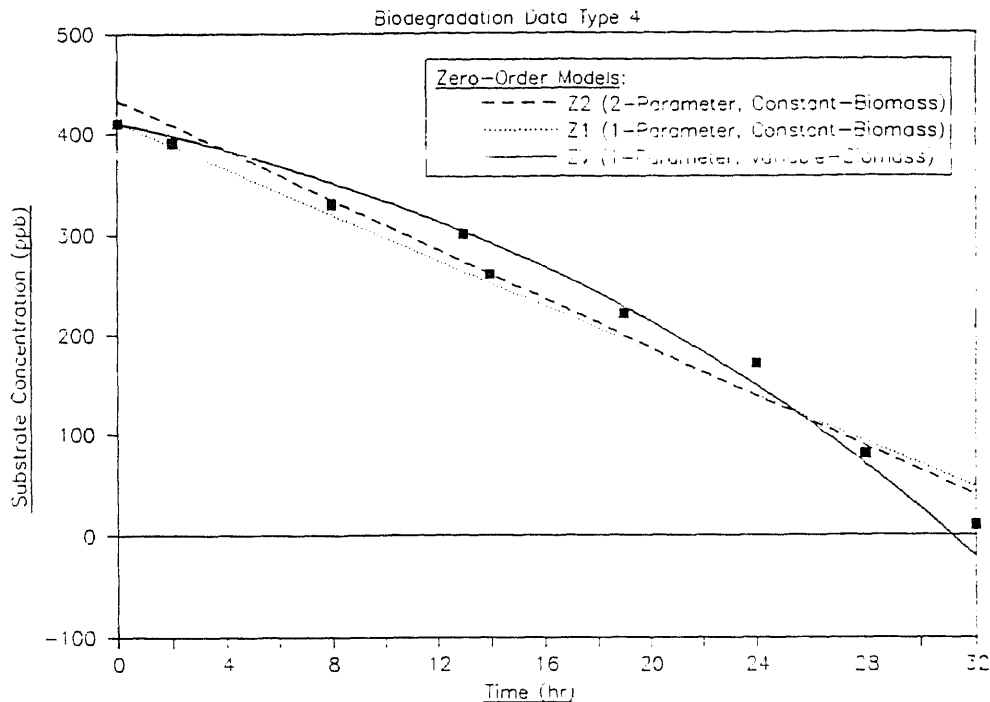
The inclusion of the substrate inhibition and endogenous decay terms (i.e.,  $S^2/K_I$  and  $k_D B$ , respectively) results in a more complex model requiring determination of the kinetic parameters (i.e.,  $\mu$ ,  $K$ ,  $K_I$ , and  $Y_c$ ;  $k_D$  was assumed a constant value of  $0.002 \text{ h}^{-1}$  by the authors) through the use of numerical methods on a mainframe computer. Whereas this model better represents this specific system than the models evaluated in this thesis, its increased complexity reduces its utility as a general purpose tool.

For data set #3 shown graphically in Figure 35, the statistically best models of those evaluated in this thesis in terms of  $\Sigma(t-t_{calc})^2$  are, in order from best to worse (refer to pages D-45 and D-46): (1) M3, (2) M2, (3) MV, (4) ZV, (5) Z2, (6) Z1, (7) FV,

(8) F2, and (9) F1. While M3 and M2 are slightly better than MV in terms of  $\Sigma(t-t_{calc})^2$ , they are much worse in terms of  $\Sigma(S-S_{calc})^2$  (refer to Figure 36). The MV model's performance is hindered somewhat by the questionable accuracy of B measurements. For higher values of  $B_0$  (i.e., 25 vs. 18.9 ppb) or lower values of  $Y_c$  (i.e., 0.1 vs. 0.136), MV performs better than M3 and M2 in all respects. Furthermore, it should be noted that both M3 and M2 regress negative values for the kinetic parameter K due to the predominantly downward bend in the data. This is analogous to the situation discussed previously in Section 6.1.1 on pages 27-31 with respect to the cases in which the Monod (constant-biomass) models yield negative values of K for zero-order data. M3 and M2 will regress negative values of K for type 4 data in cases where the downward bend predominates versus the opposing first-order curvature. Depending on the given data set, M3 and M2 can both yield positive or negative values of K; it is also feasible that situations may arise where M3 and M2 will yield K values of opposite sign. Because the constant-biomass Monod models are unable to model the downward bend in type 4 data without the regression of negatives values for K, they are as a general rule inappropriate for type 4 data.

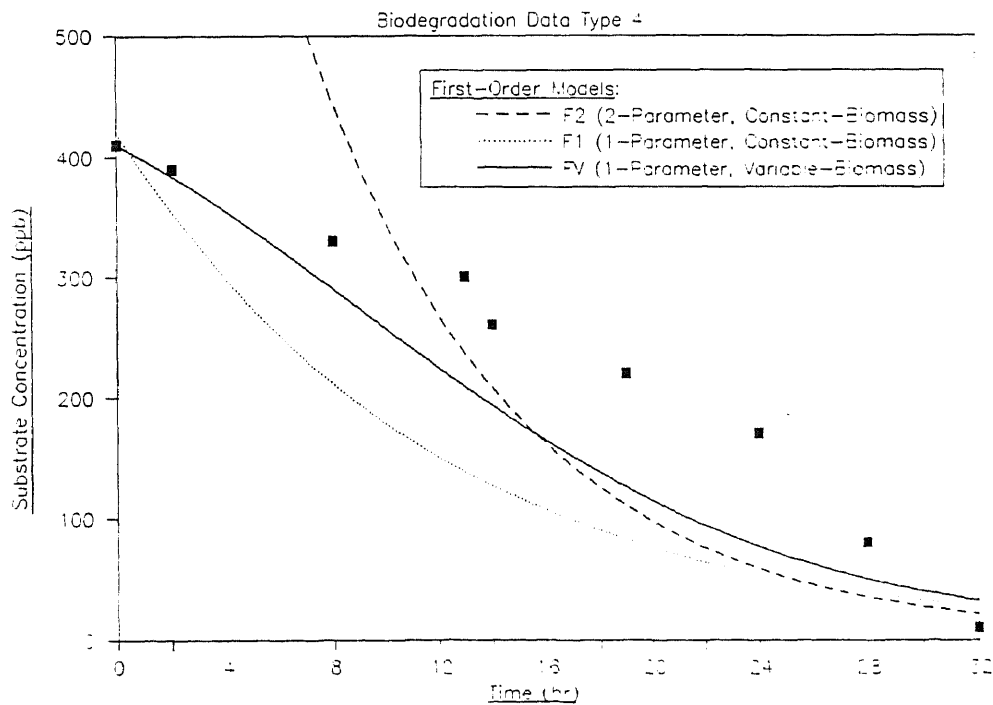
Figures 37 and 38 present all of the zero- and first-order models, respectively, for the same data set shown in Figure 36. In both cases, the variable-biomass curves are better than the corresponding constant-biomass models, but all are notably worse than the MV curve shown in Figure 36.

Figure 37



Source : Klecka, G.M. & Maier, W.J. (data set #3 on pages D-45 & D-46)

Figure 38

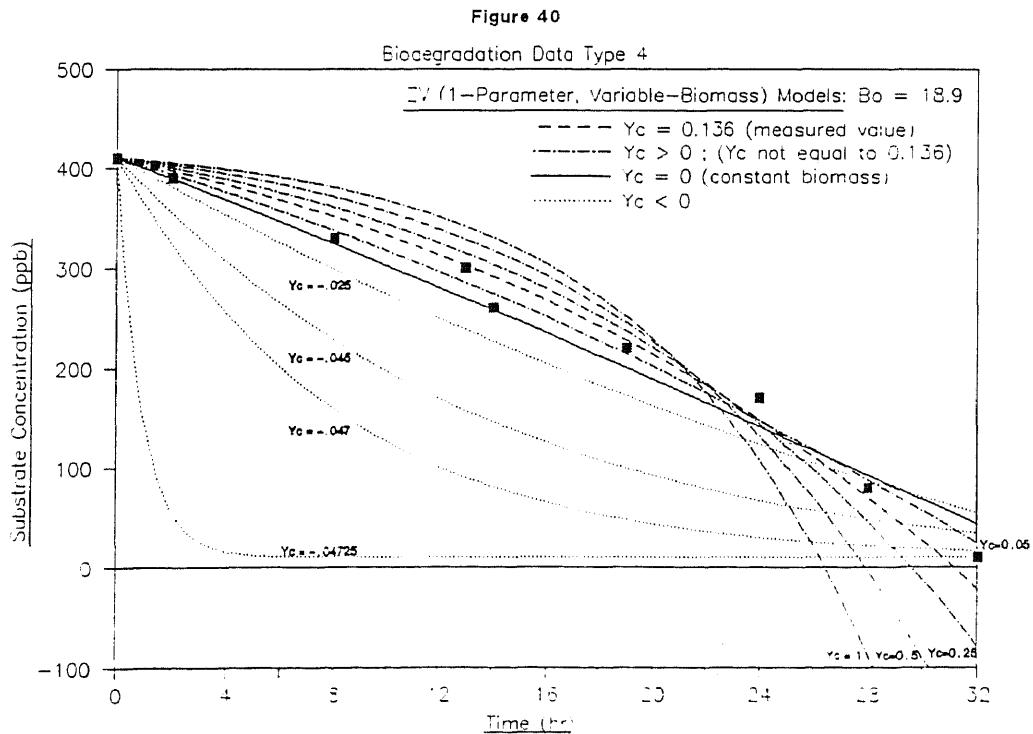
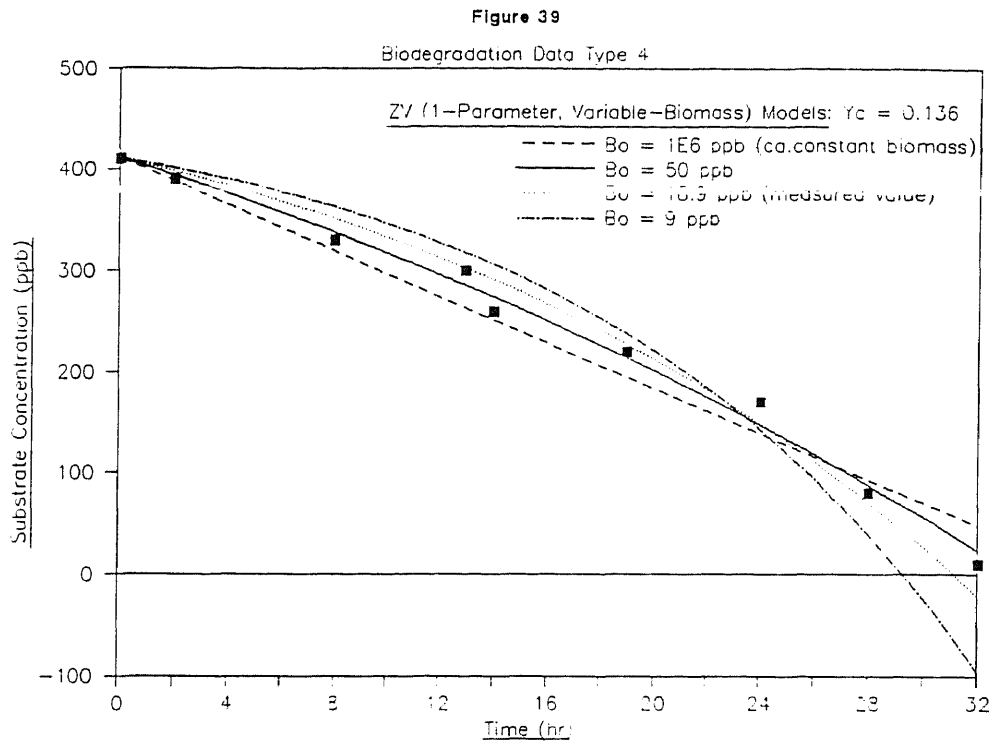


Source : Klecka, G.M. & Maier, W.J. (data set #3 on pages D-45 & D-46)



Whereas the constant-biomass, zero-order models are incapable of fitting any curvature (slope =  $dS/dt$  = constant =  $-k$ ), Figure 37 shows that ZV does not have this restriction because of the assumption of exponential biomass growth (slope =  $dS/dt$  =  $-k_0 B_0 \exp(k_0 Y_c t)$ ; this expression reduces to  $dS/dt = -k_0 B_0 = -k$  when  $Y_c=0$  or, in other words, when constant-biomass conditions prevail). As in the constant-biomass case, the variable-biomass model predicts complete degradation after a finite period of time (i.e., x-intercept at  $t = (1/k_0 Y_c) \ln(1 + Y_c S_0 / B_0)$ ) beyond which negative values of  $S$  are predicted. It is because of the inability of ZV to model the inflection in type 4 data that it is inappropriate in virtually all cases, especially when extrapolating.

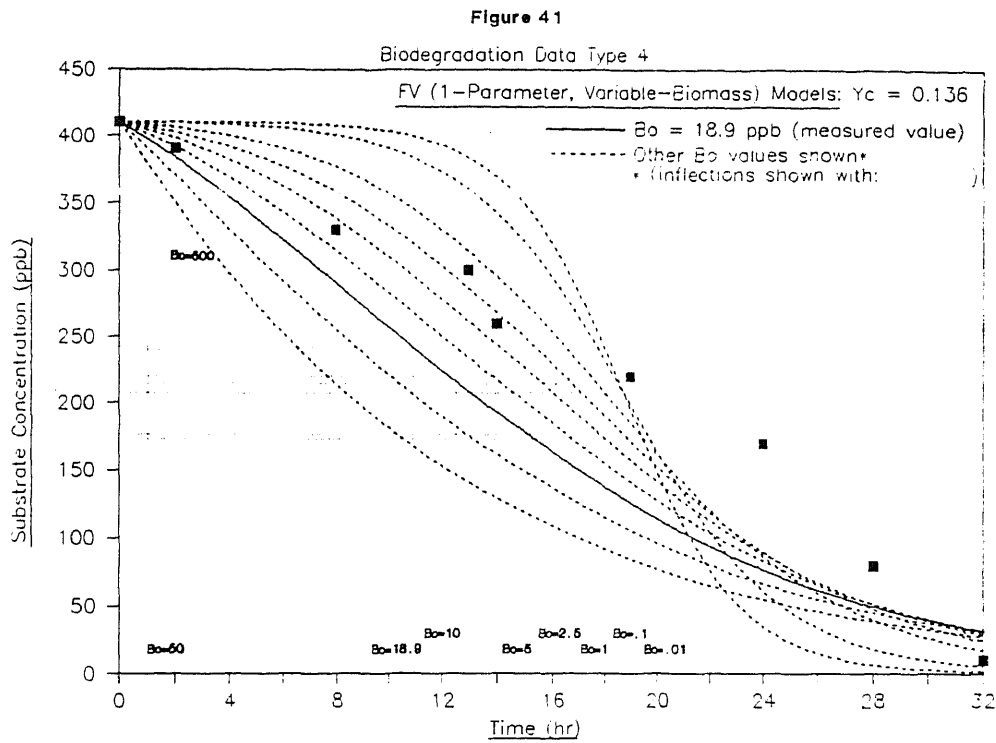
Figures 39 and 40 show the effects of the values of  $B_0$  and  $Y_c$ , respectively, on the performance of the ZV model for the same data set presented in Figures 35 through 38.  $B_0$  is always a positive value with theoretical limits of 0 and 1,000,000 ppm. Figure 39 shows that ZV approaches constant-biomass behavior as  $B_0$  increases. As  $B_0$  decreases, the variable-biomass effect increases (i.e., the predicted initial biodegradation rate decreases, approaching the limit of 0, while the rate of change becomes more dramatic, approaching the limit of an almost vertical drop). Figure 39 shows that a much better fit of the data is obtained with the ZV model when a value of 50 ppb is used in place of the measured value of 18.9 ppb for  $B_0$ . This does not



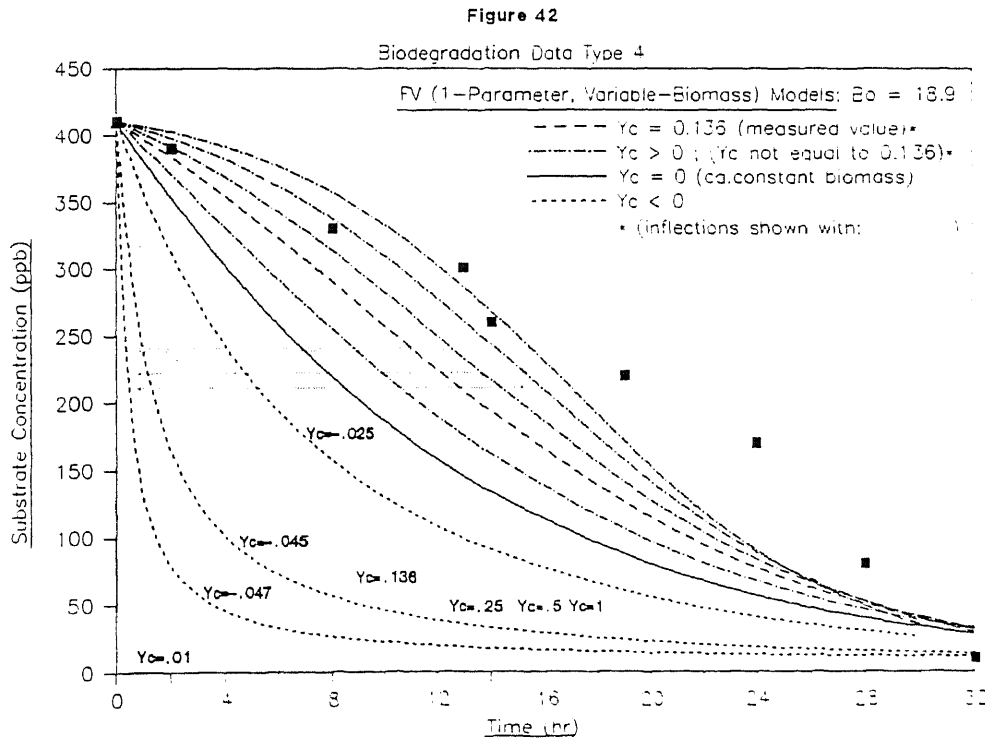
necessarily mean, however, that the measured value of  $B_0$  is inaccurate. Rather, the value of  $Y_c$  may be more suspect.

Figure 40 shows the effect of the value of  $Y_c$  on the regressed ZV curves. Whereas  $Y_c$  is typically expected to have values of between 0 and 1, negative values have in certain anomalous situations been observed to occur and they were therefore examined here, even if only for esoteric purposes. The higher the value of  $Y_c$ , the greater the variable-biomass effect observed; constant-biomass behavior is approached as  $Y_c$  approaches 0. As values of  $Y_c$  drop below 0, the curvature of the ZV model is reversed resembling that of positive nth-order kinetics. ZV curves for negative values of  $Y_c$  can be predicted only for the case in which  $Y_c$  is greater than  $-B_0/(S_0-S)$ . This is mathematically due to the requirement that the function  $f = (B_0 + Y_c S_0 - Y_c S)/B_0$  be greater than zero in order for the logarithm of the function to be real. Physically, this is due to the fact that  $B$  cannot in reality be negative. It should be noted that the sensitivity of the variable-biomass models to  $Y_c$  is dependent on  $B_0$ , and vice versa, as the two parameters are interrelated.

Figure 38 shows FV to be the best of the first-order models evaluated. Unlike F1 and F2, FV exhibits a downward bend with an inflection at  $t = (1/(k_0(B_0 + Y_c S_0))) \ln(Y_c S_0/B_0)$  followed by the more conventional first-order curvature. This effect is more readily apparent in Figures 41 and 42 which show the response of the FV curves to changes in  $B_0$  and  $Y_c$ , respectively, for this data set. These figures both show



Source: Klecka, G.M. & Maier, W.J. (data set #3 on pages D-45 & D-46)

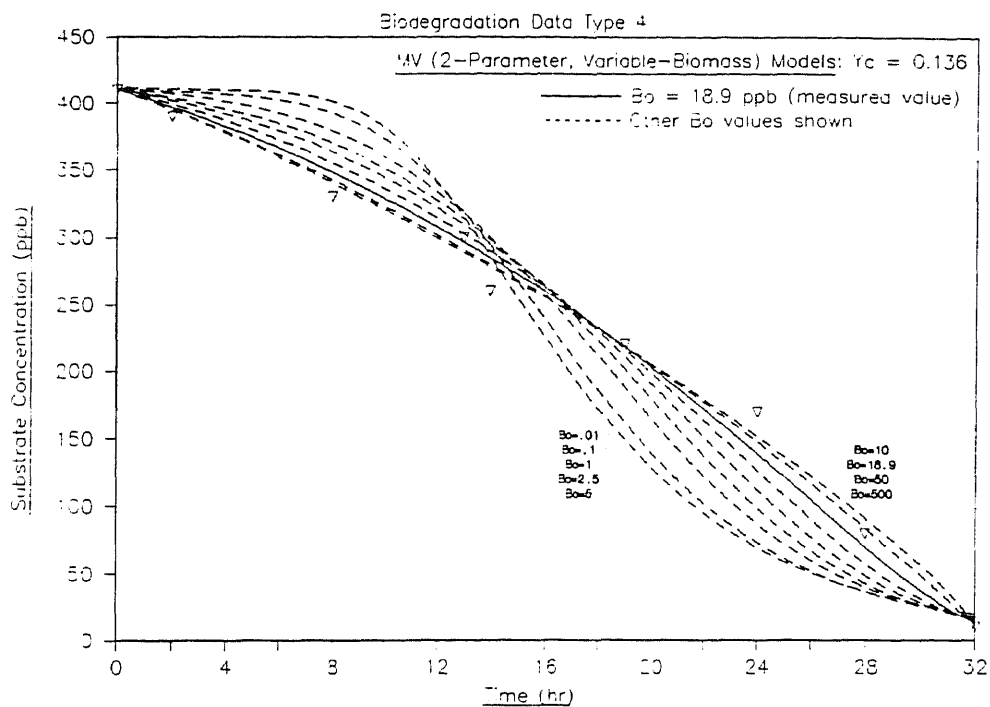


Source: Klecka, G.M. & Maier, W.J. (data set #3 on pages D-45 & D-46)

increased variable-biomass effects (i.e., initial biodegradation rate approaches 0 while the ultimate biodegradation rate approaches infinity) as either  $B_0$  is decreased or  $Y_c$  is increased. Conversely, constant-biomass behavior (i.e., the F1 curve) is approached as  $B_0$  increases or  $Y_c$  decreases. The two figures show that, as either  $B_0$  increases or  $Y_c$  decreases, the inflection occurs at correspondingly lower values of  $t$  until such a point as it drops below zero and is no longer visually apparent (note: for negative values of  $Y_c$ , inflections do not exist at all).

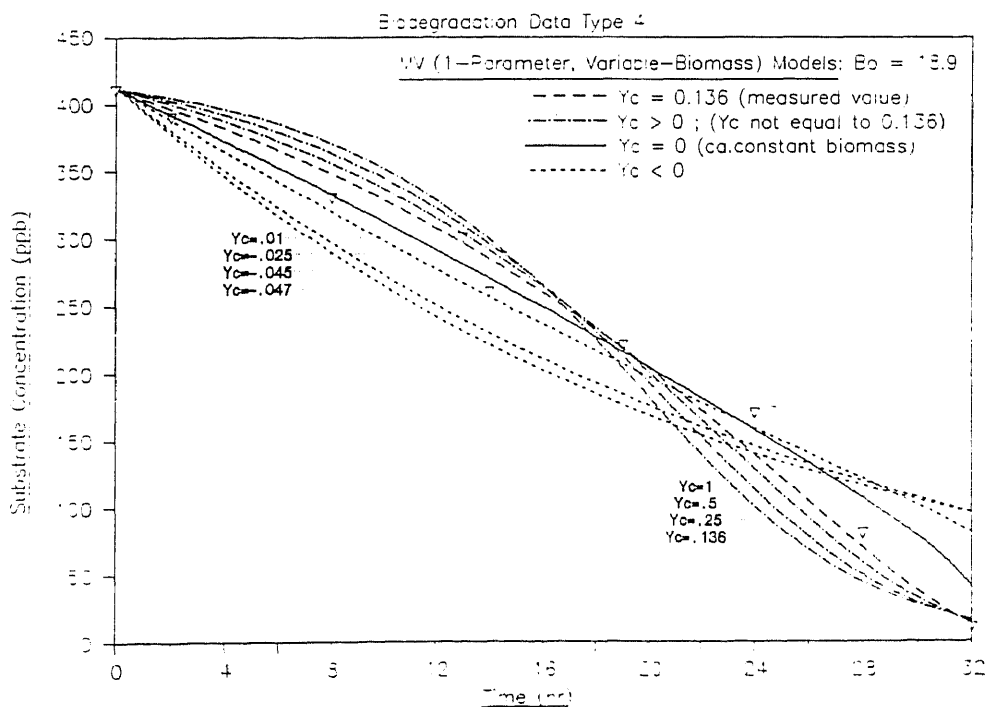
Figure 42 also shows that negative values of  $Y_c$  result in the prediction by FV of the equivalent of a greater-than-first-order drop. As stated previously for the ZV models, FV curves can be predicted only for negative values of  $Y_c$  in which  $Y_c$  is greater than  $-B_0/(S_0-S)$ . It is apparent from Figures 41 and 42 that the FV model is especially sensitive to the values of  $B_0$  and  $Y_c$ . Qualitatively, the FV model possesses similar characteristics to the MV model and it may be difficult to classify a data set as either FV or MV based on visual inspection of the data alone. The MV model, however, is visually and statistically much better for type 4 data, and is also much less sensitive to errors in  $B_0$  and/or  $Y_c$  as seen in Figures 43 and 44 which show the corresponding MV curves for the same values of  $B_0$  and  $Y_c$  shown in Figures 41 and 42, respectively. The MV curves have the ability to better model a more gradual transition from initial to maximum biodegradation rate compared to the FV curves. As a side note, Figure 44 shows the MV model

Figure 43



Source: Klecka, G.M. & Maier, W.J. (data set #3 on pages D-45 & D-46)

Figure 44



Source: Klecka, G.M. & Maier, W.J. (data set #3 on pages D-45 & D-46)

to lose its inflection and resemble the FV model when negative values of  $Y_c$  are used (although the effect is less pronounced for the MV model).

While the MV model is less sensitive in terms of fit than the FV model to errors in  $B_0$  and  $Y_c$ , it may result in regression of negative values of  $K$  for some data sets if  $B_0$  and  $Y_c$  do not correspond to a sufficient enough variable-biomass effect. For example, the MV model yields negative values for  $K$  in Figure 43 when  $B_0$  is greater than 35 ppb and in Figure 44 when  $Y_c$  is less than 0.08. To avoid this problem with the MV model inadequately representing type 4 data, it is crucial that biomass measurements be accurate.

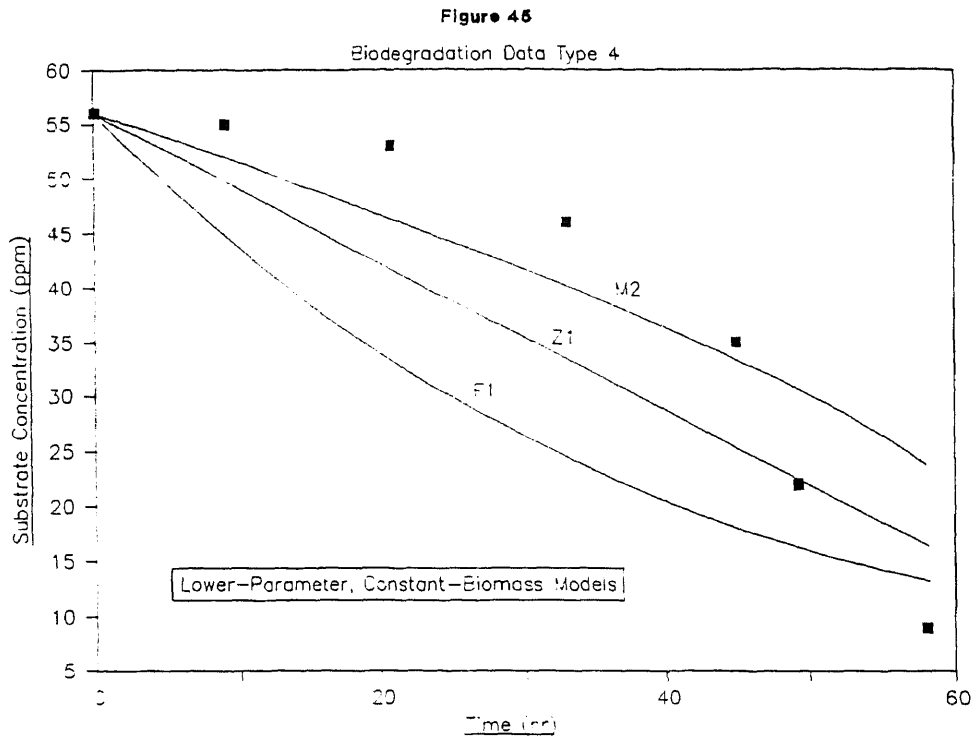
Data set #4 (shown in Figure 35) is analogous in behavior to data set #3 which was discussed extensively above. Data set #4, however, covered a lower  $S$  range which, in turn, resulted in a higher relative percentage error in  $S$  measurements. This increased uncertainty resulted in reduced confidence in model selection as the statistical differences between the model types are less significant (refer to pages D-47 and D-48). The variable-biomass models still, however, perform better than the constant-biomass models, with MV being the best. Note that the M2 is the only one of the three Monod models to regress a negative value of  $K$  for this data set. While the values of  $B_0$  and  $Y_c$  appear reasonably accurate for this case, they are not optimum in that they do not result in the best possible fits for the three variable-biomass models evaluated. Furthermore, the values of  $B_0$  and  $Y_c$  which

yield the best fit for one of the variable-biomass models (e.g., MV) does not necessarily yield the best fit for the others (e.g., FV and ZV).

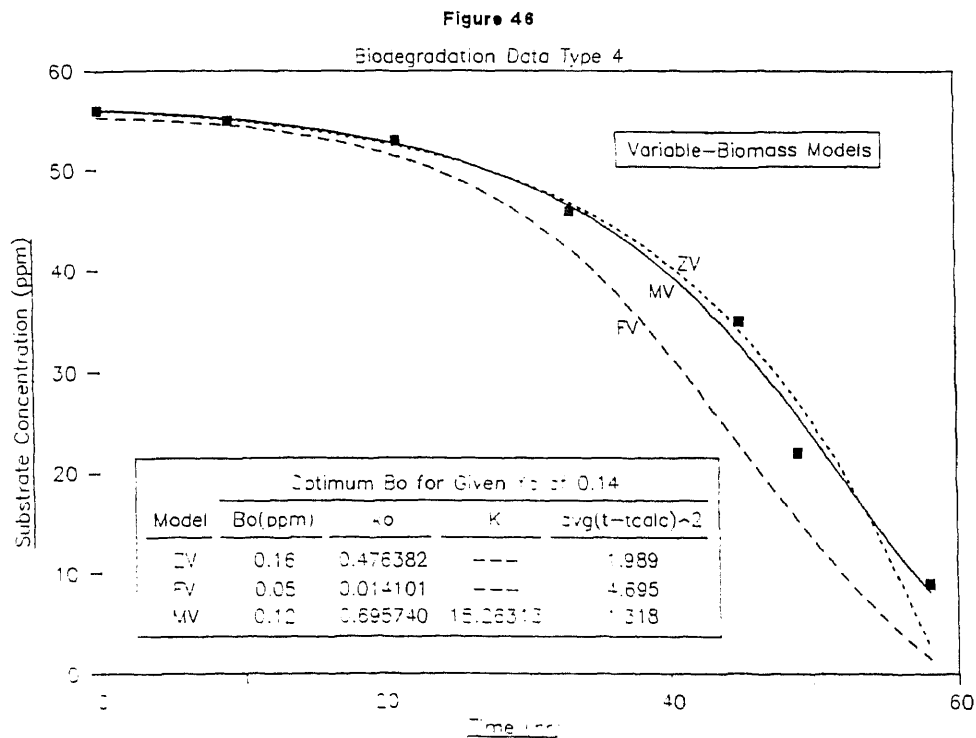
Papanastasiou and Maier studied the mutual-inhibition effect of a glucose/2,4-D, dual-substrate system of which Figure 45 presents the  $S$  vs  $t$  curve for one of the two substrates (i.e., 2,4-D). The authors fit their data using a modified Monod equation that incorporated a term to account for inhibition by alternative substrates as described by Yoon, et al.<sup>5</sup> Whereas this model is better than the models evaluated in this thesis for predicting the behavior of this specific dual-substrate system, it may be too complex and specific to be of value as a general purpose tool.

The lower-parameter, constant-biomass models are graphically shown in Figure 45 to be terrible in representing the data set which apparently exhibits a very strong variable-biomass effect. The authors, however, did not provide sufficient biomass data (i.e.,  $Y_c$  was given but  $B_0$  was not) to assess the variable-biomass models, and hence, the corresponding tabulation for this set is not given in Appendix D. Figure 46, however, graphically shows the three variable-biomass models (i.e., MV, ZV and FV) for the cases in which  $B_0$  was selected (i.e., with  $Y_c$  being set at the given value) so as to minimize the value of  $\Sigma(t-t_{calc})^2$ . The data set is best represented by the MV model. While the ZV model is reasonable over the range considered, significant errors will result when extrapolating outside the range due to the inability of ZV to represent the inflection and subsequent first-order





Source: Papanastasiou, A.C. & Maier, W.J. (data set #3 shown on page D-57)



Source: Papanastasiou, A.C. & Maier, W.J. (data set #3 shown on page D-57)

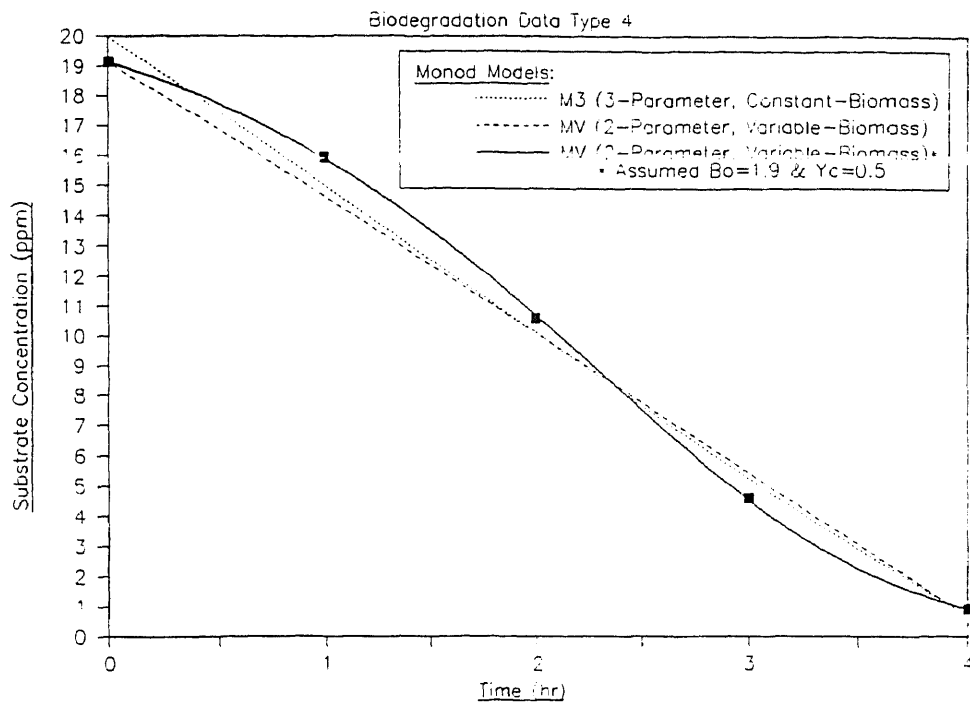
effect. The FV model, while characteristically correct in terms of general curvature, is less flexible than the MV model and has greater difficulty fitting data which are not very nearly first order.

The optimum values of  $B_o$  shown in Figure 46 are slightly different for each of the three models. The value for MV is intermediate between those for ZV and FV, which is to be expected since the data is intermediate between zero and first order. In each of the three cases,  $B_o$  is very low which is characteristic of such a system with a pronounced variable-biomass effect. It is highly unlikely that the author's measurements would have provided such a low value for  $B_o$  since the culture was an activated sludge with an expected total biomass concentration of 1000-5000 ppm. None of the commonly-used, biomass-measurement techniques accurately differentiate active from inactive biomass, especially when the active cells are at such a low level relative to the total population.

It should be noted that the M2 and M3 models both regressed negative values of  $K$  for the data set presented in Figures 45 and 46. While the MV model yielded a positive value of  $K$  for the case shown in Figure 46, a negative value would be obtained for higher values of  $B_o$  where the variable-biomass effect is sufficiently diluted such that the model is forced to regress a negative  $K$  in order to fit the predominantly downward bend in the given data set.

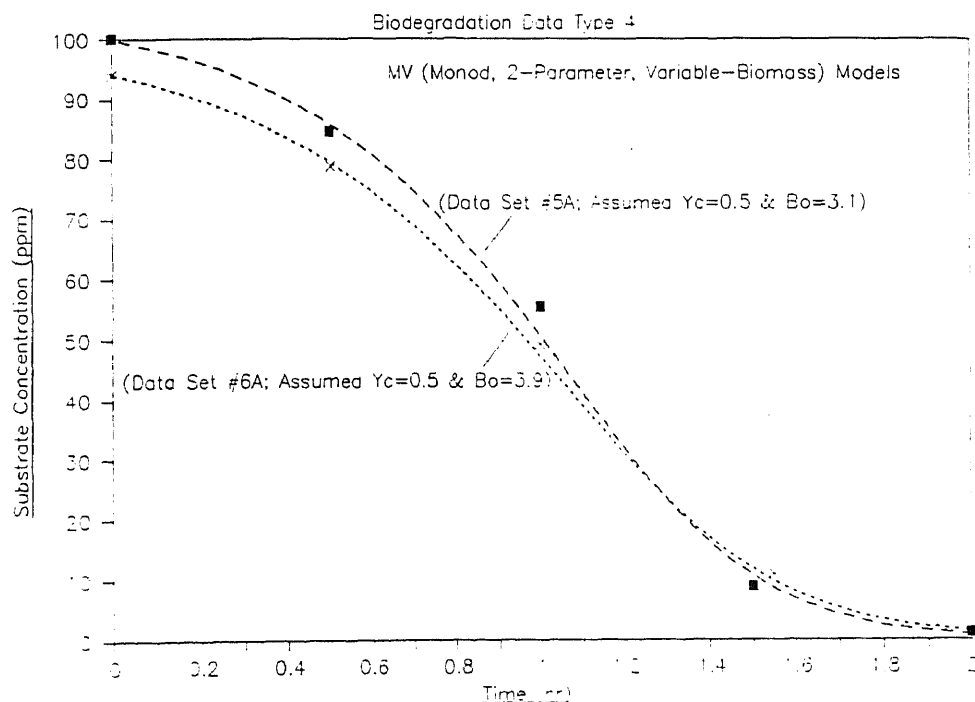
In addition to the 4 data sets discussed thus far in this section, 3 more of the 124 mixed-culture systems evaluated in this thesis were classified as type 4 (refer to Figures 47 and 48). Figure 47 presents the M3 and MV models regressed from the available data shown on pages E-10 and E-11, as well as an MV model for which an optimum value of  $B_o$  (i.e., such that  $\Sigma(t-t_{calc})^2$  was minimized) was selected for an assumed value of 0.5 for  $Y_c$ . The former two are notably worse than the latter. The data summaries on pages E-10 and E-11 show the Monod models in general to be little better than the zero-order models. M2 and MV, in particular, yield negative values of  $K$ , while only M3 regresses a positive value. The optimum MV curve shown in Figure 47 also yielded a positive value of  $K$ . The reason for the poor performance of the MV model shown on page E-11 is the inaccurate biomass measurements which resulted, for one thing, in an unrealistically high value of  $Y_c$ . Of more importance than the  $Y_c$  value is the fact that the  $B_o$  value is a measure of the total biomass concentration and not the viable biomass level. As a result, the  $B_o$  value is excessively high accounting for the predicted variable-biomass effect being much less than that observed. For example, the predicted increase in biomass concentration is only 8.9% for the case shown on page E-11 versus 480% for the optimum fit shown on Figure 47.

Figure 47



Source : Colish Thesis (data set #3 shown on pages E-10 & E-11)

Figure 48



Source : Naik Thesis (data sets #5A & #6A on pages E-70 & E-73, respectively)

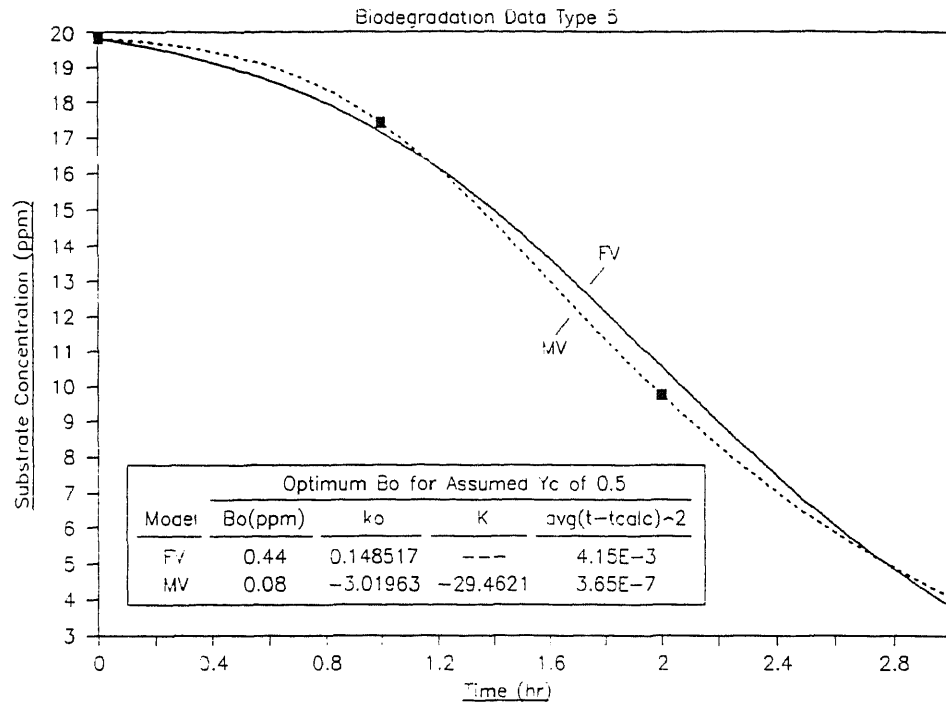
Figure 48 presents two data sets from the Naik thesis for the same system with the optimum MV curves shown. The variable-biomass models were not evaluated utilizing actual biomass measurements because of the inherent nature of the multiple substrate system involved which made determination of the substrate-specific parameters of  $B_0$  and  $Y_c$  impractical.

#### 6.1.5 Date Type 5 (First-Order, Variable Biomass)

This biodegradation data type can be considered a limiting case of data type 4 in which  $S$  is kinetically limiting relative to  $B$ . This data type is well represented by the FV model with Figures 41 and 42 in Section 6.1.4 visually presenting the characteristic features of this data type as well as the effect of the parameters  $B_0$  and  $Y_c$  on the regressed FV curves.

Figure 49 shows the data set from pages E-12 and E-13 to be reasonably well represented by a hypothetical FV model (i.e.,  $Y_c$  assumed to be 0.5 and  $B_0$  was then selected so as to minimize  $\Sigma(t-t_{calc})^2$ ). The performance of this FV model is significantly better than the models on pages E-12 and E-13. The M2 and M3 models regress negative values of  $K$  to fit the predominantly downward bend in the data while the MV model does the same because of the inherent inaccuracy of the measured biomass data (i.e., "total", not "viable", biomass was measured) which results in an underprediction of the observed variable-biomass effect (e.g., the measured biomass increased by only 5.2% over the range of  $S$  consumed while the optimum FV curve predicts an 1800% increase in order to model the observed effect).

Figure 49



Source : Colish Thesis (data set #4) ; refer to pages E-12 & 13

Figure 50

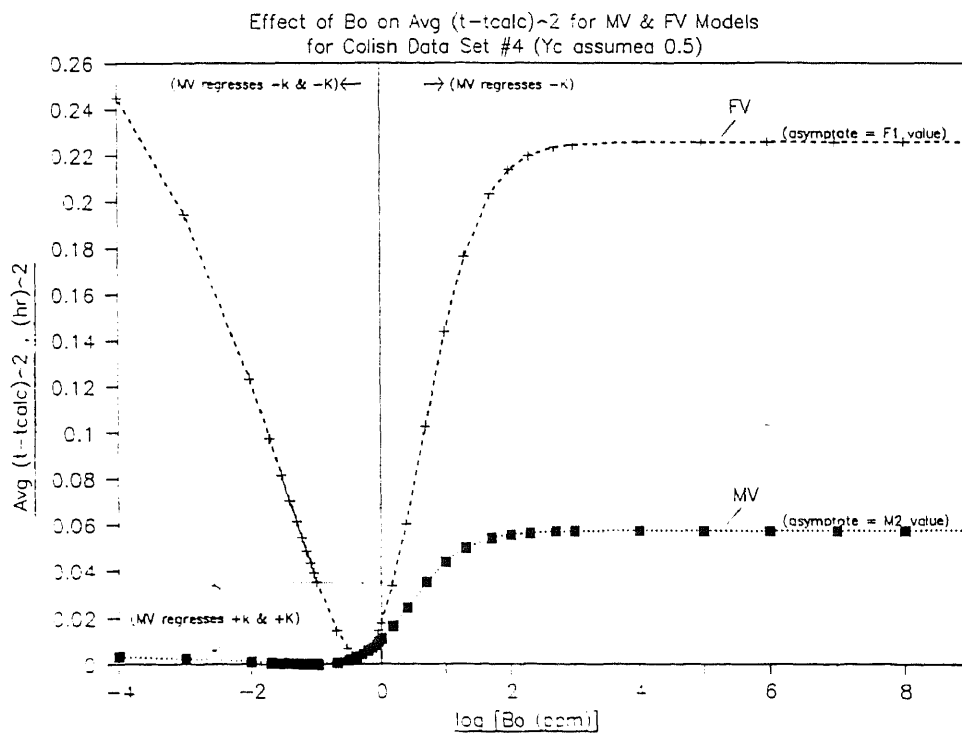


Figure 49, in addition to the hypothetical FV model, shows a hypothetical MV model to fit the data perfectly. The MV model, however, regresses negative values of both  $k$  and  $K$  because of the data being interpreted by the model as greater than first order for the values of  $B_0$  and  $Y_c$  used. Figure 50 graphically presents the effect of  $B_0$  on the fit of the data (shown in Figure 49) in terms of the statistic  $\Sigma(t-t_{calc})^2$  for both the FV and MV models. This plot again demonstrates the point made previously in Section 6.1.4 that the FV model is much more sensitive to errors in biomass measurements than MV. The MV model, however, is also extremely sensitive to inaccurate biomass measurements from the perspective that negative kinetic parameters may be regressed (refer to Figure 50 to see the relatively small range of  $B_0$  values for which MV regresses positive values of both  $k$  and  $K$ ). The data set in Figure 49 is classified as FV and not MV because the optimum FV curve results in a lower  $\Sigma(t-t_{calc})^2$  than the optimal MV for which positive kinetic parameters are obtained. The MV model will always result in a better fit of type 5 data than the FV because of the additional degree of freedom provided by the kinetic parameter  $K$  in the former. Because type 5 data will always possess some experimental error, however, the MV model has an approximately equal probability of regressing either both positive (if the data is interpreted by MV as being less than or equal to first order) or both negative values (if the data is interpreted by MV as being greater than first order) for  $k$  and  $K$ ,

provided the biomass data are accurate. As a result of this, the FV model is preferred over the MV for type 5 data.

Figures 51 and 52 present two more examples of type 5 data with the optimal MV and FV curves shown in each case. In both cases the Monod model is statistically slightly better. In Figure 51, MV yields positive rate constants while in Figure 52 it yields negative rate constants. Figure 51 shows the optimal MV curve to be that for the limiting case of constant biomass.

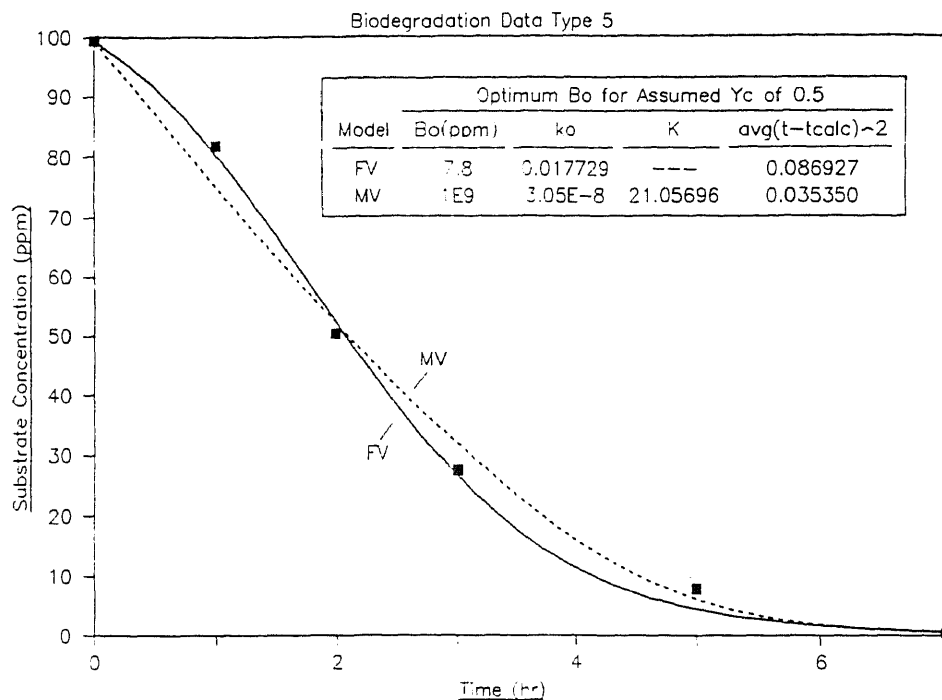
#### 6.1.6 Data Type 6 (Zero-Order, Variable Biomass)

This biodegradation data type is a limiting case of type 4 data where B is kinetically limiting relative to S (i.e.,  $S \gg B$ ) over the entire range of S covered. These autocatalytic reactions are terminated before the biodegradation rates reach their maximum value (i.e., no inflection is obtained). This data type is well represented by the ZV model with Figures 39 and 40 in Section 6.1.4 visually presenting the characteristic features of this data type as well as the effect of the parameters  $B_0$  and  $Y_c$  on the regressed ZV curves.

As mentioned previously in Section 6.1.1, most industrial problems involve removal of pollutants down to very low levels where S is limiting relative to B and first-order curvature is apparent. Operation under substrate-limiting conditions is also desired in activated-sludge, wastewater treatment facilities so as to minimize bacterial growth (i.e., via endogenous respiration) since disposal of excess sludge is both

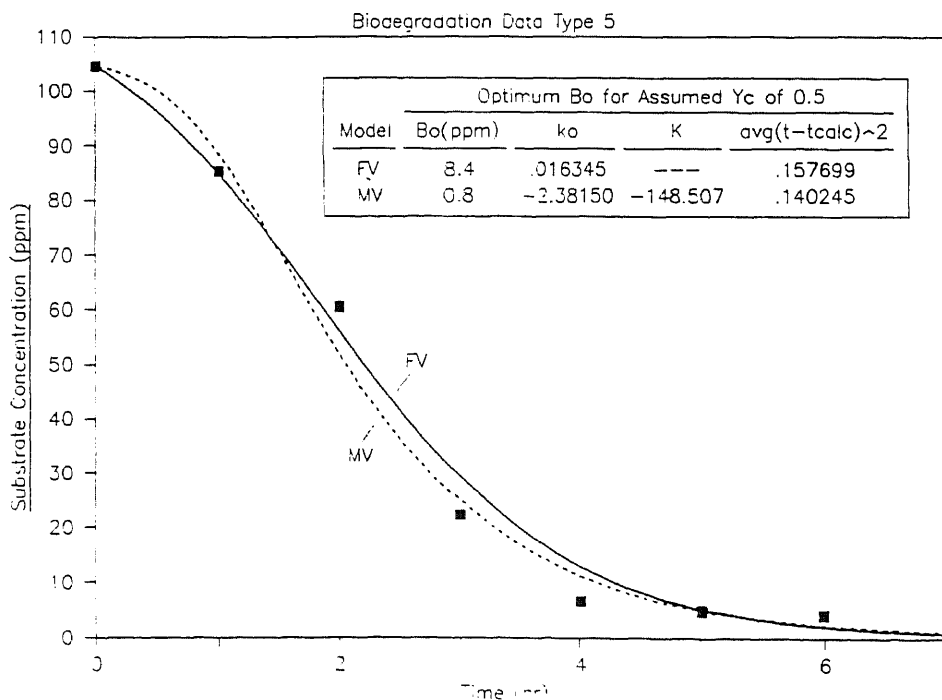


Figure 51



Source : Naik Thesis (data set #4A) ; refer to page E-67

Figure 52

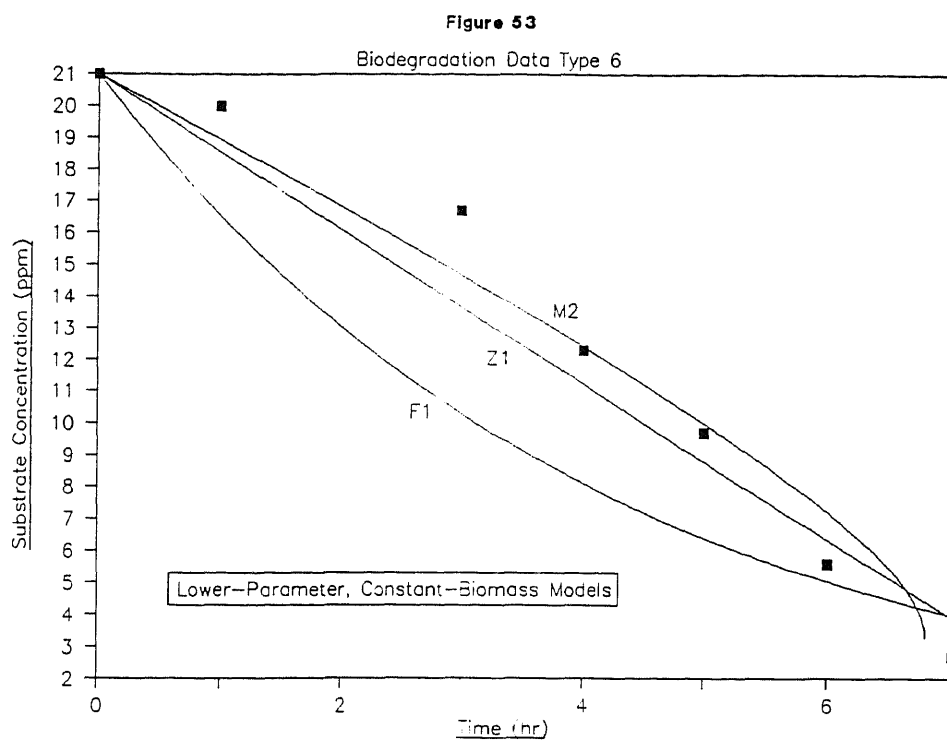


Source : Pak Thesis (data set #10) ; refer to page E-106

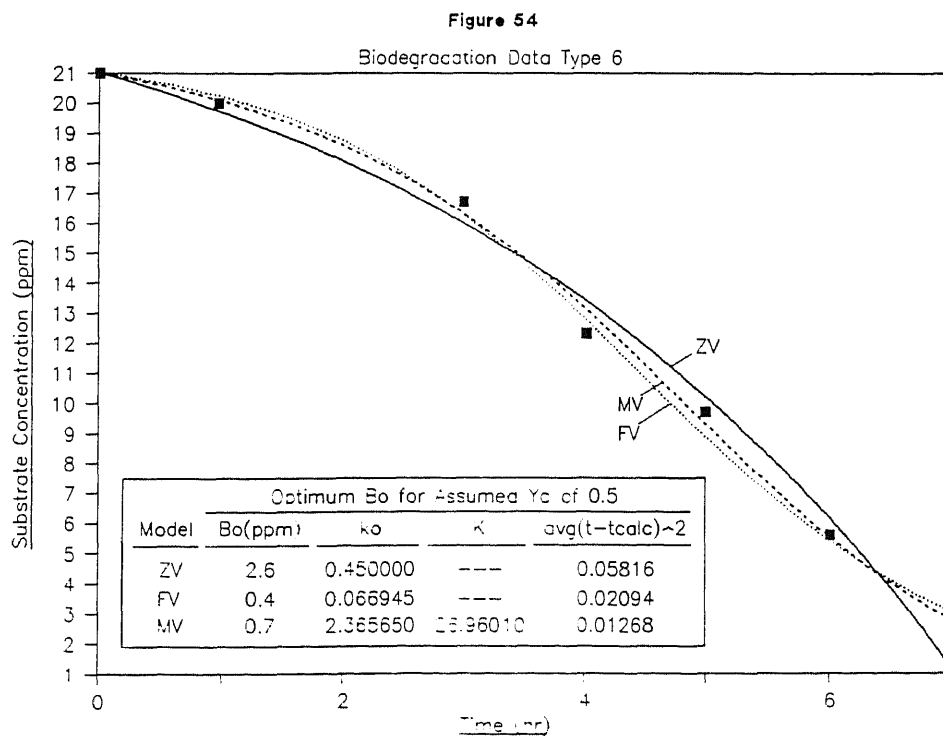
problematic and costly. It is, therefore, natural that most laboratory studies would logically operate under similar conditions. This is exactly what was observed in the cases studied in this thesis as only 2 of the 116 mixed-culture systems were categorized as type 6 data.

Figure 53 presents the first of the two data sets categorized here as type 6, along with the corresponding lower-parameter, constant-biomass models from page E-39. None of the constant-biomass models are appropriate for data of this sort. Z1 and Z2 cannot model any curvature, while F1 and F2 predict curvature opposite to that actually observed. Whereas M2 and M3 can model the downward bend inherent in data of this type, they do so via the regression of negative values of K and are, therefore, not valid.

Figure 54 shows the same data set to be well-fitted by all three variable-biomass models. Each of the three curves are hypothetical and represent the best possible fit for each model type for the case in which  $Y_c$  is assumed to have a value of 0.5. Because of the scatter in the data and the lack of information as to the magnitude of the experimental error, it is not possible to select one (with any high degree of confidence) as being the "correct" depiction of reality. While the Monod is statistically best (as always), its regression is sensitive to the accuracy of biomass measurements with respect to obtaining



Source : Gonnabathula Thesis (data set #10B) ; refer to page E-39

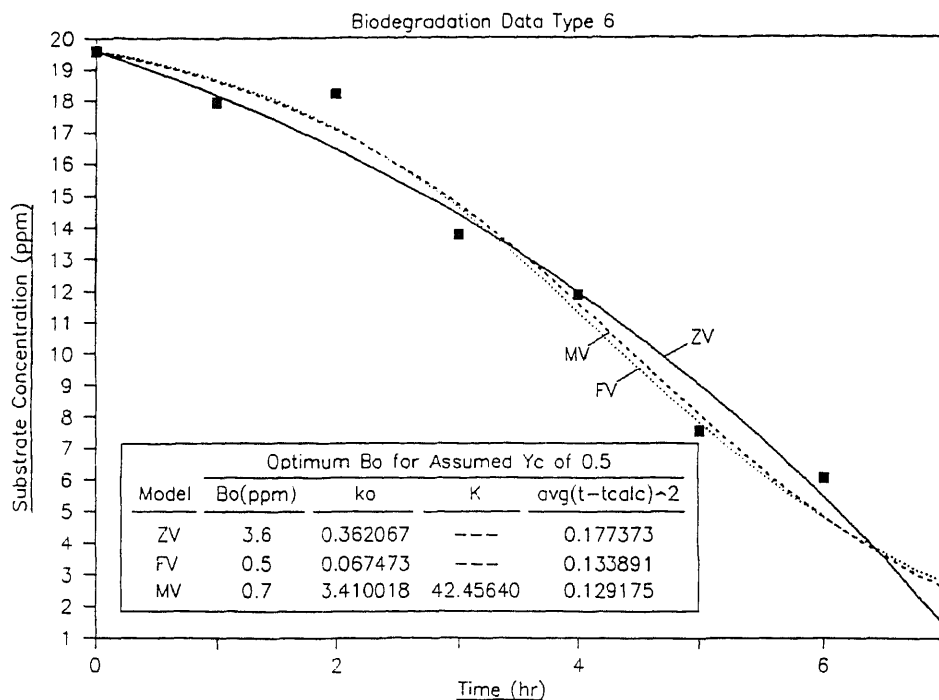


Source : Gonnabathula Thesis (data set #10B) ; refer to page E-39

positive rate constants (as mentioned previously in Sections 6.1.4 and 6.1.5); negative values of  $K$  are obtained in this case for values of  $B_o > 4$  ppm and negative values of both  $k$  and  $K$  are obtained for values of  $B_o \leq 0.3$  ppm. Furthermore, while MV provides a statistically better fit than ZV, it may be overfitting the experimental error in the data and not necessarily better representing reality. For both of these reasons, the ZV model is generally preferred over the MV for type 6 data, but only over the range of  $S$  and conditions covered (i.e., ZV is not appropriate for extrapolation because of an imminent transition to first-order kinetics). The FV model happens to fit this data set nearly as well as the MV. As mentioned previously (refer to Figure 50), however, the FV model is extremely sensitive to the accuracy of biomass measurements. For values of  $B_o$  not immediately near the optimum, the FV model becomes significantly worse than the ZV.

Figure 55 presents the only other data set categorized as type 6. None of the constant- or variable-biomass models regressed on pages E-8 and E-9 are very good representations of the system. While the constant-biomass models suffer for the same reasons as stated on page 90 for the data set shown in Figure 53, the variable-biomass models suffer from inaccurate biomass measurements. Colish measured bulk biomass and not the active bacterial population. The substrate used (i.e., o-chlorophenol) is relatively resistant to biodegradation and, as such, only a small percentage of the overall sludge would be expected to be able to utilize it.

Figure 55



Source : Colish Thesis (data set #2) ; refer to pages E-8 & E-9

Figure 56

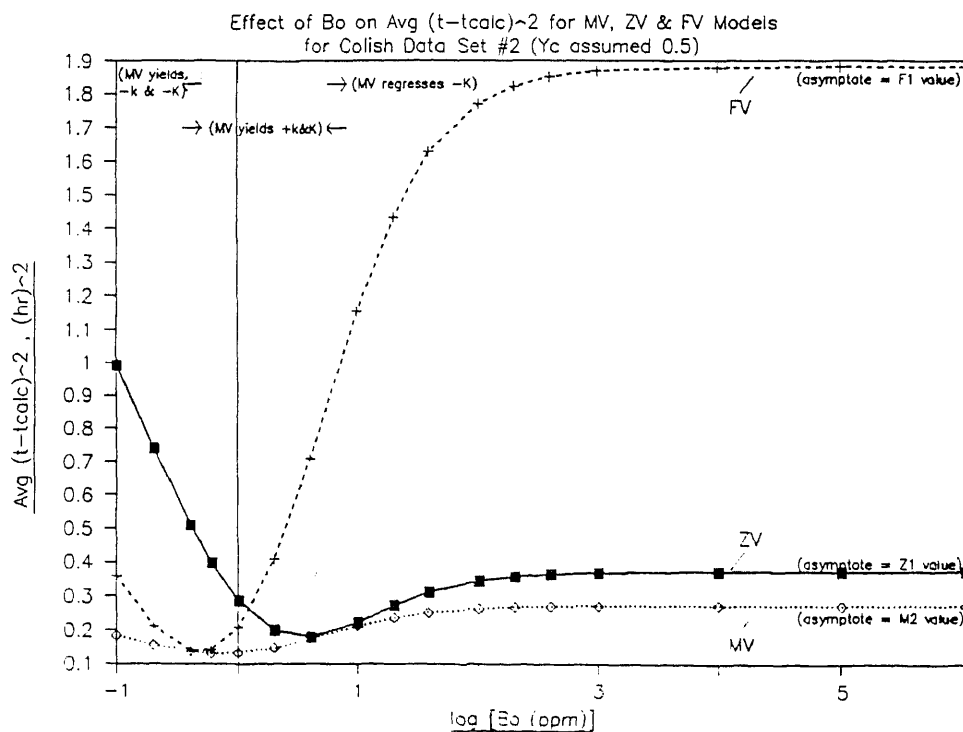


Figure 56 shows the effect of  $B_0$  on the fit of the three variable-biomass models to the data set presented in Figure 55 for an assumed  $Y_c$  value of 0.5. While the Monod is statistically best over the entire range, it requires accurate, viable-biomass measurements in order to regress positive coefficients. FV also requires accurate, viable-biomass measurements in order to obtain a good fit. ZV is less sensitive to errors in  $B_0$  and is only slightly worse than MV over the practical range of interest and is, therefore, preferred for type 6 data. Figure 55 graphically presents the optimum fit for each of the three variable-biomass models from Figure 56 (i.e., for the value of  $B_0$  which minimizes  $\Sigma(t-t_{calc})^2$ ). All are feasible for the data set presented. Selection of the "true" model for this data set is hindered by the data scatter and lack of information from the author as to the magnitude of the experimental error.

#### 6.1.7 Data Type 7 (Lag followed by Biodegradation)

Biodegradation data type 7 consists of the broad group of  $S$  vs.  $t$  curves where lags are apparent. The portions of the curves following the lags may be characteristic of any of the first six biodegradation types discussed thus far. The lag represents the acclimatization of micro-organisms to a substrate. During the lag, the bacterial cells have long generation times and are characterized by zero growth rates. Nutrients are taken into the cells and the mass of bacteria increases as the amount of enzymes and nucleic acid increases. Once a

sufficient amount of the substrate-specific enzymes are generated, biodegradation takes place as discussed in the previous sections. The length of the lag period is variable (i.e., it is dependent on the size and degree of adaptation of an inoculum to its new environment). Lags are common in batch-reactor studies where the sludges are not sufficiently acclimated to the substrates.

None of the models evaluated in this thesis are theoretically capable of depicting the often abrupt transition from lag to utilization characteristic of this data type. The ability of the models studied herein to reasonably well fit data sets of this type is largely dependent on the length of the lag relative to the overall biodegradation time (e.g., the shorter the lag, the better the potential fit). For the case of the constant-biomass models, the higher-parameter versions are notably better than the corresponding lower-parameter versions because of their ability to average the error, in the initial portion of the  $S$  vs  $t$  data, resulting from the models' inherent inabilities to properly fit the lag. The variable-biomass models are potentially better (depending, in part, on the accuracy of  $B_0$  and  $Y_c$ ) than the constant-biomass models for data of this type, but their dependency on accurate biomass measurements limits their practical usefulness. The best approach for data of this type is to disregard the lag and fit the remaining biodegradation portion of the  $S$  vs  $t$  data. The appendices, however, present the results for each complete data set as

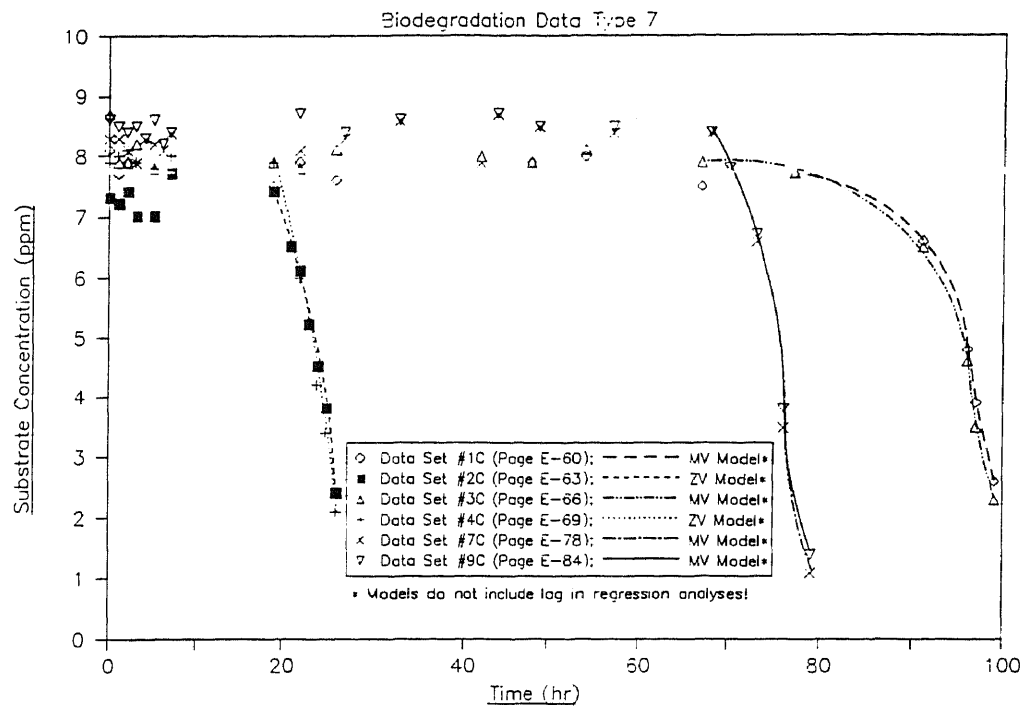
given by the corresponding sources; the segregation approach (i.e., separation of the lag from the data set before performing the kinetic analysis) is demonstrated graphically within this section for comparative purposes only. As stressed previously, it is imperative that the system (i.e., biomass composition/concentration, etc.) be well-defined in order for the kinetic analyses to be useful for design purposes.

The lag measured on laboratory scale in batch reactors is often not regarded as a concern in large-scale facilities, which consist of continuous reactors operating under the assumption of steady state. Knowledge of the activity of the acclimated sludge for a specific substrate (which is typically derived from batch reactor studies), however, is crucial to the design and performance of these continuous units. Furthermore, the assumption of steady state is not always valid, as the feedstock to wastewater-treatment facilities may vary significantly and, as such, specific information on the unsteady-state behavior of a sludge in response to these changes is necessary to ensure proper operation.

The commonality of the occurrence of lags in batch-reactor studies is apparent in this thesis as 44 of the 124 data sets reviewed (for mixed-culture systems) possess them. Figures 57 through 66 show all 44 of the data sets along with the models best deemed to represent them.

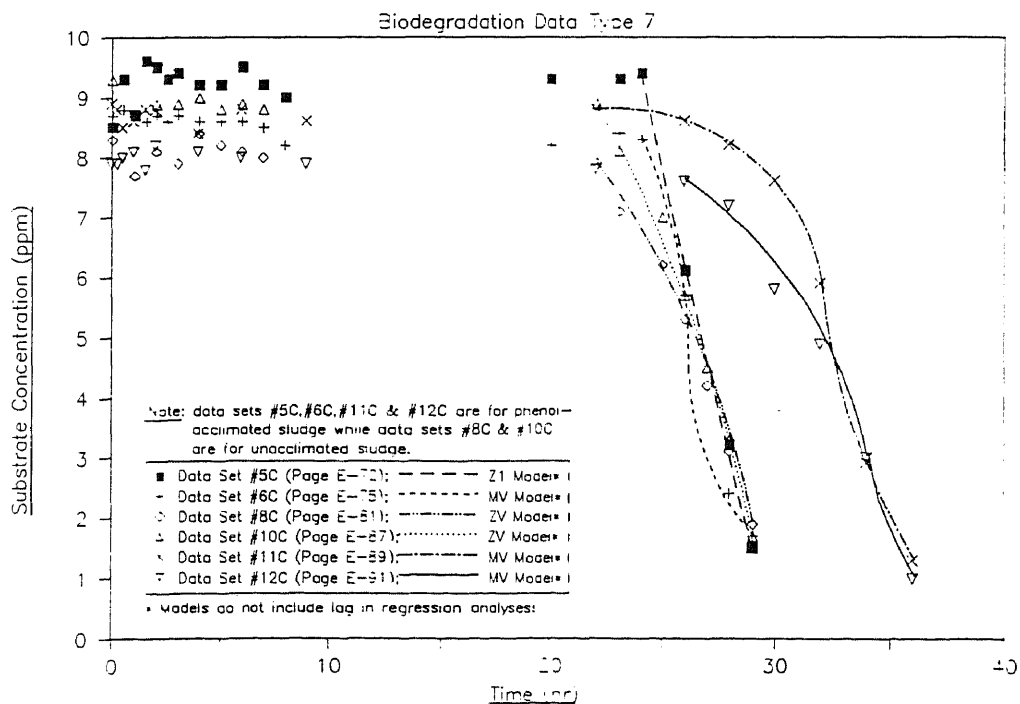


Figure 57



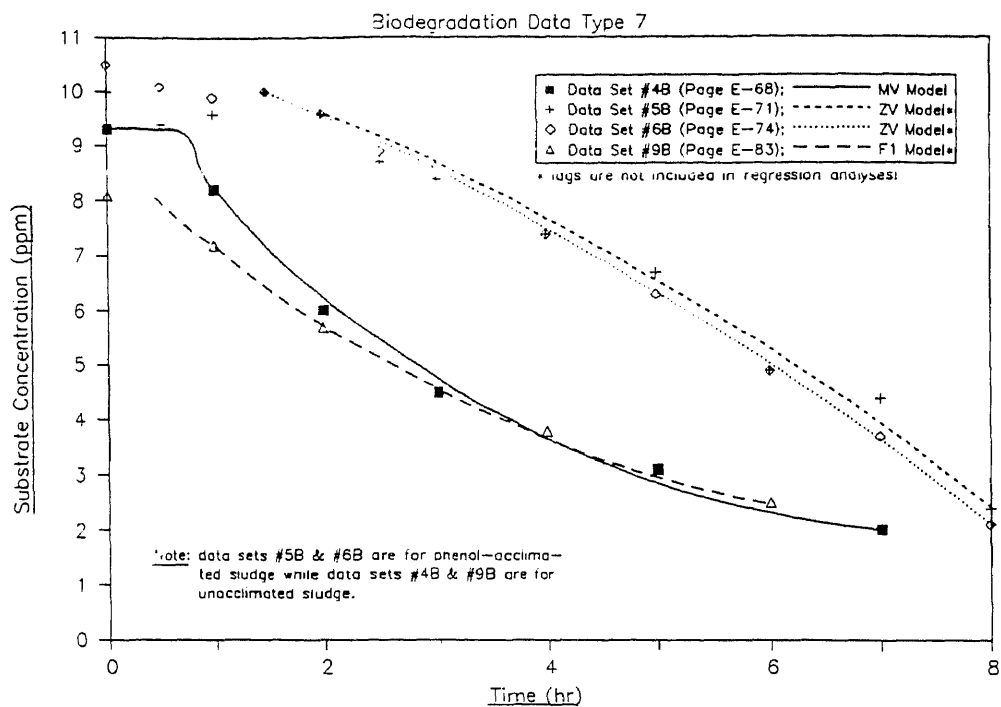
Source: Naik Thesis (2,6-dichlorophenol in unacclimated sludge)

Figure 58



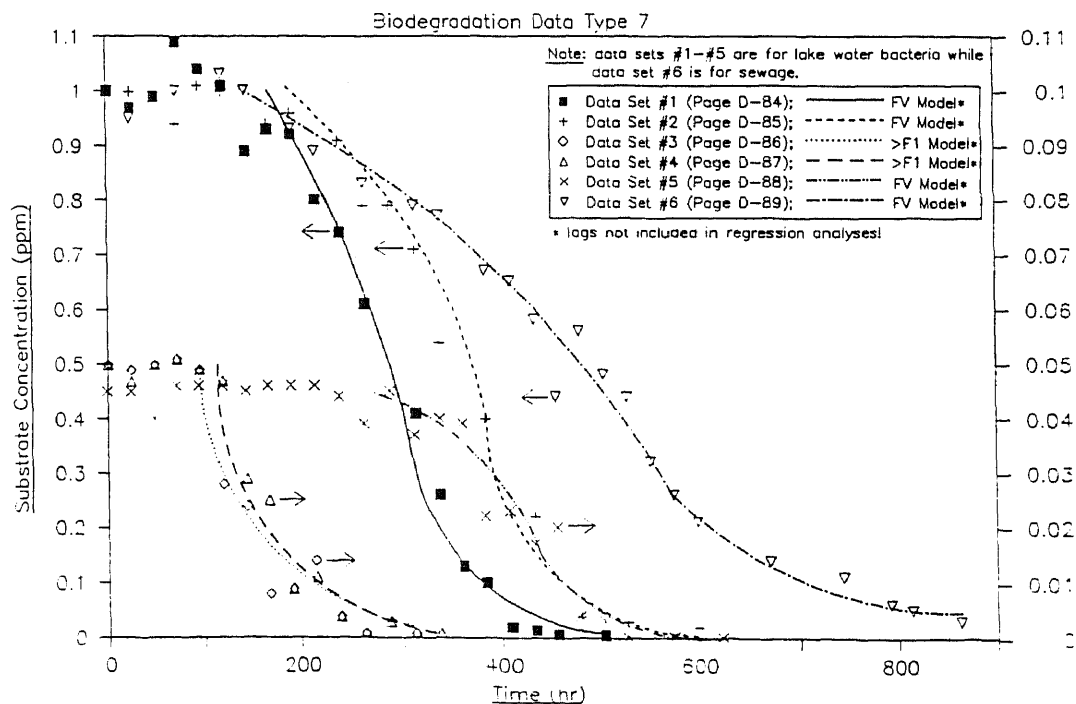
Source: Naik Thesis (2,6-dichlorophenol as substrate)

Figure 59



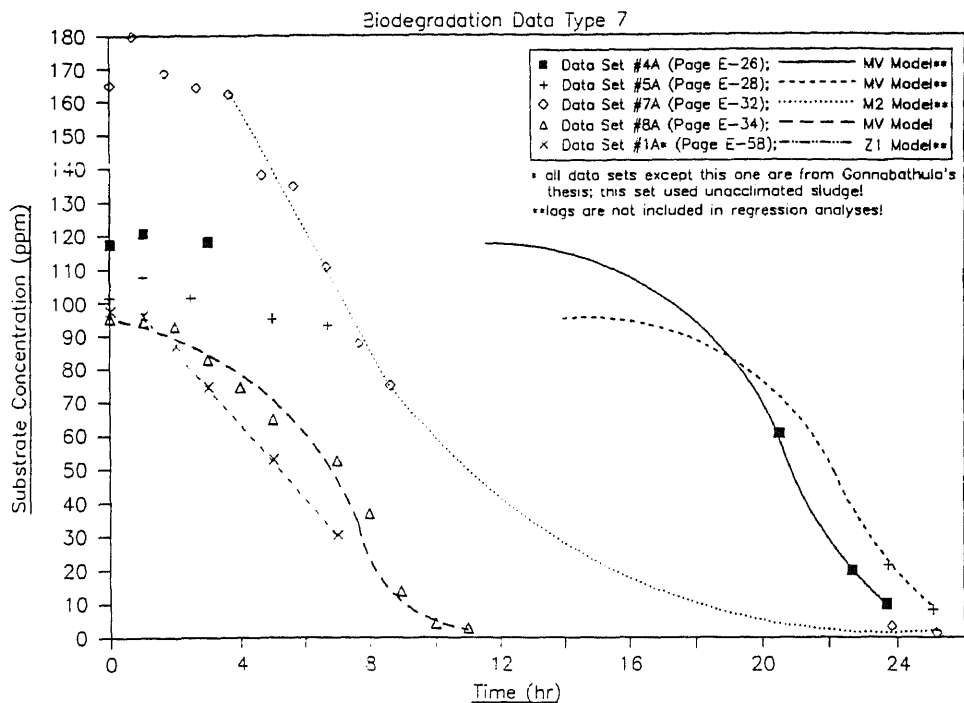
Source : Naik Thesis (nitrobenzene substrate)

Figure 60



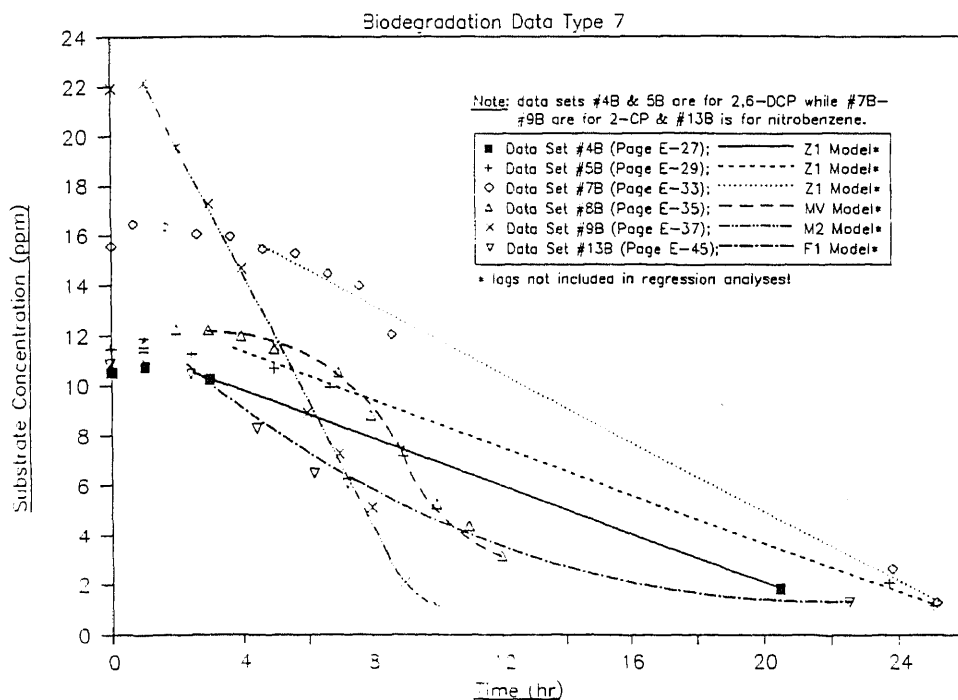
Source : Yordy, J.R. & Alexander, M. (N-nitrosodimethylamine as substrate)

Figure 61



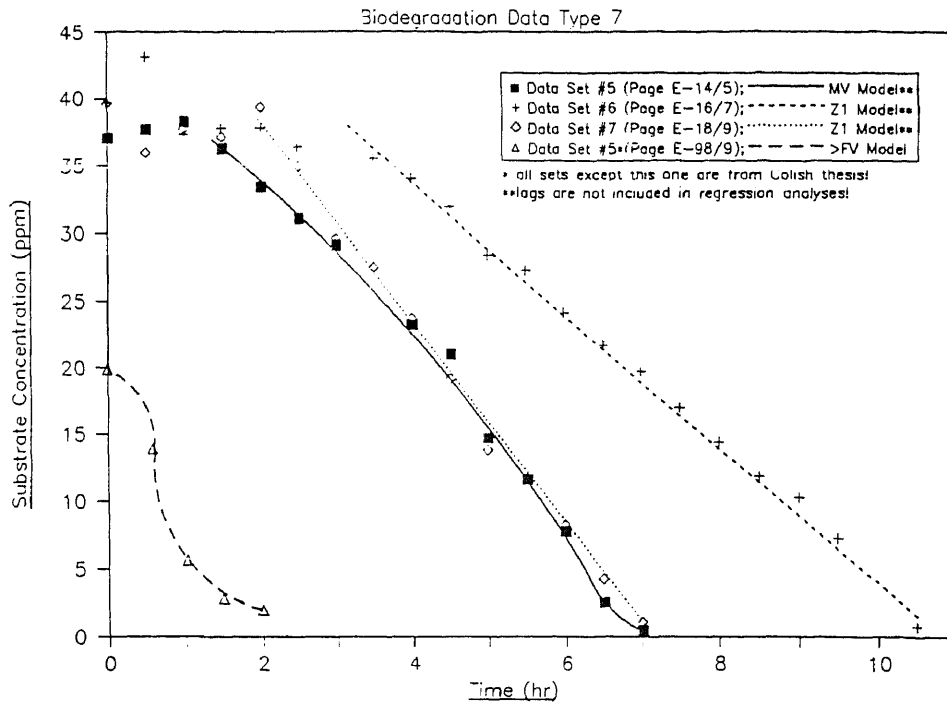
Source : Gonnabathula & Naik Theses (phenol as substrate in mlss)

Figure 62



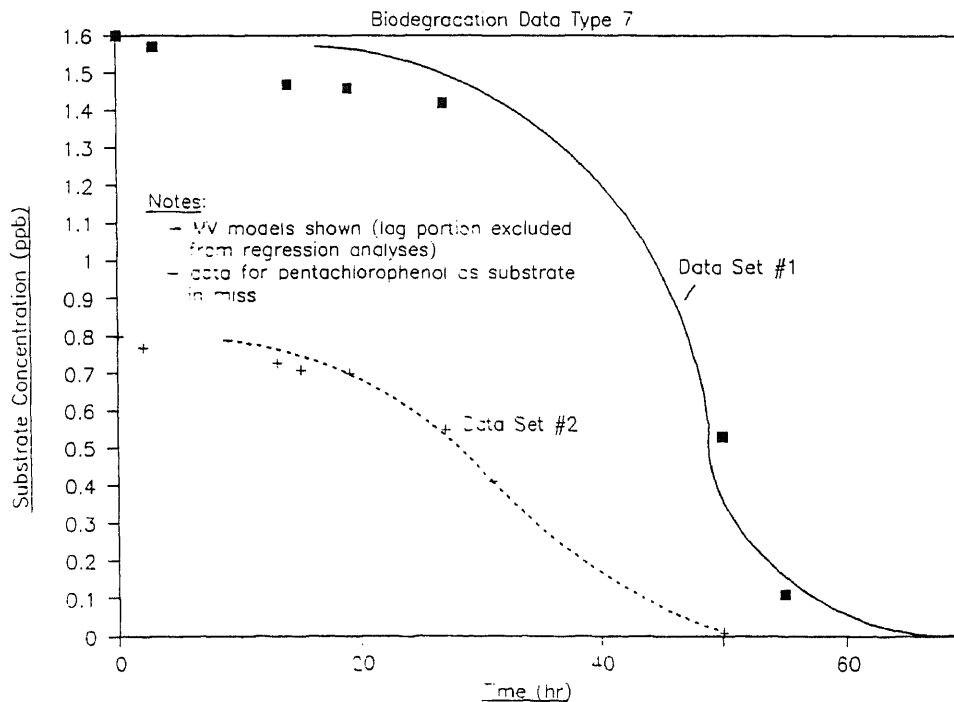
Source : Gonnabathula Thesis (aromatic substrates in mlss)

Figure 63



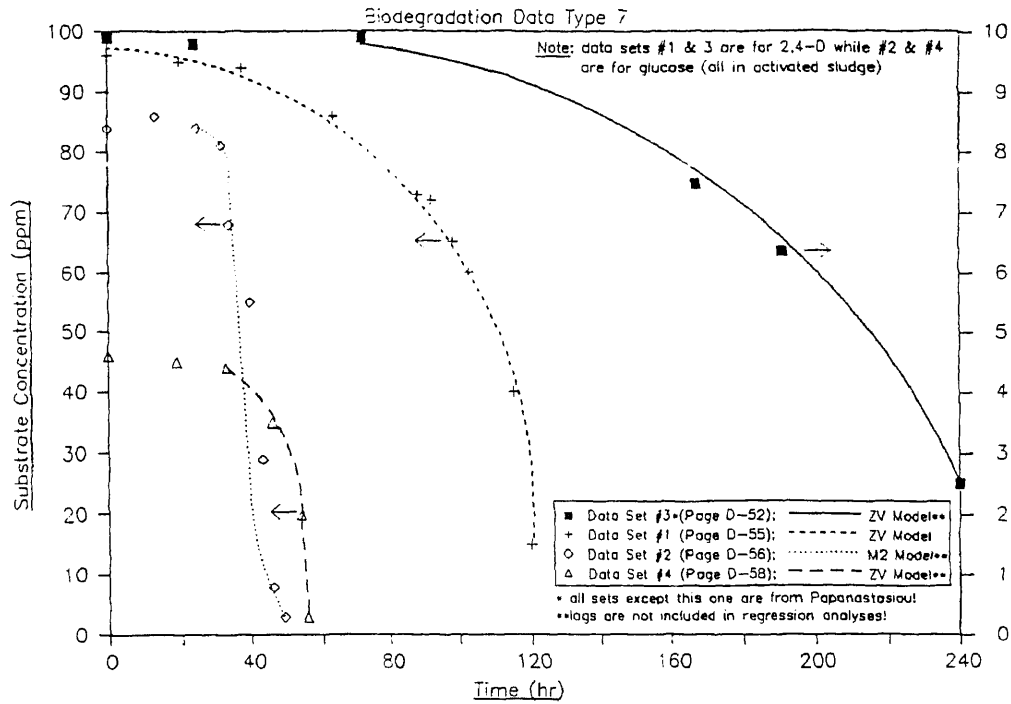
Source : Colish & Pak Theses (2-chlorophenol as substrate in mlss)

Figure 64



Source : Hecker, G.M. & Maier, W.J. data sets #1 & #2 on pages D-41 thru 44)

Figure 65



Source : Papanastasiou, A.C., et al and Liu, D., et al.

Figure 66

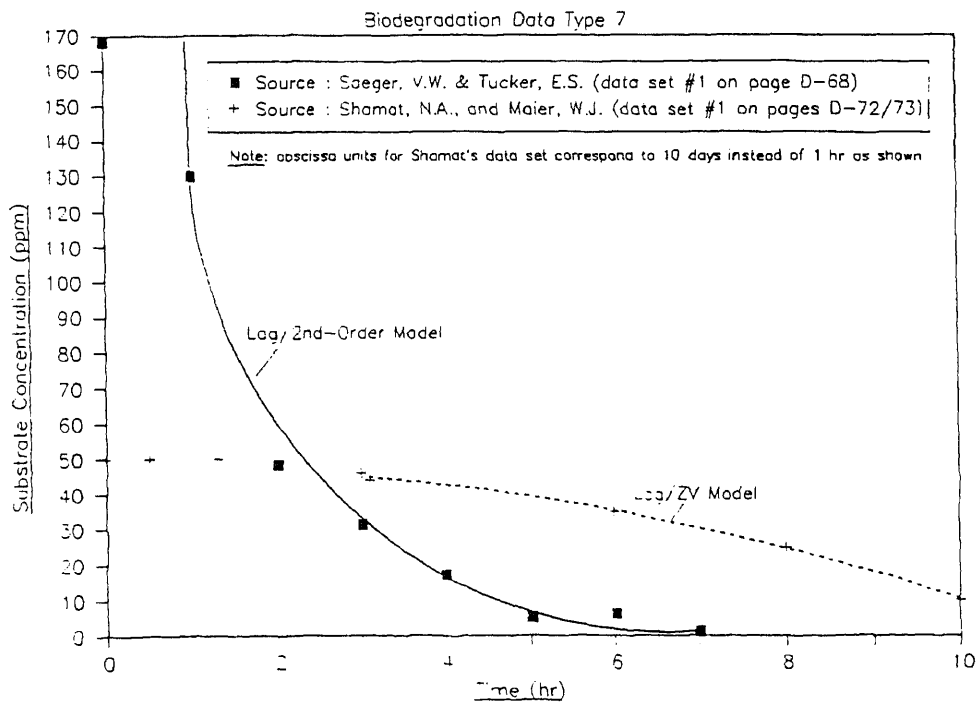


Figure 57 shows six data sets for the same system (i.e., 2,6-dichlorophenol in unacclimated sludge) to yield widely different results in terms of lag length and model type. The differences are attributed to subtle differences between the systems which were not adequately defined by the experiments. For example, "unacclimated" sludges used in data sets #1C and #3C were then used (after partial acclimation in those runs) in data sets #2C and #4C, respectively; even though the sludges had partially acclimated, their classification as "unacclimated" sludge had not changed even though the performance characteristics of the sludges apparently had. The reproducibility between data sets #1C and #3C, and between data sets #2C and #4C (which were both virtually duplicate runs), was excellent. Data sets #7C and #8C were also replicate runs but involved a different co-substrate from the other four runs, thereby accounting for the observed difference in results.

In all six data sets shown in Figure 57, the length of the lags are too long relative to the biodegradation portions to allow adequate representation of the complete data sets by any of the models studied in this thesis. The constant-biomass models are worse than for biodegradation data type 4 (refer to Figure 45 in Section 6.1.4). In all cases, M2 and M3 regress negative values of K to try to fit the downward bend in the data. The zero-order models are unable to model the bend in the data while the first-order models predict curvature opposite to that observed. The variable-biomass models are also unable to adequately

represent the precipitous transition from lag to utilization observed in these sets. As such, the data could only be suitably fitted by models studied in this thesis when the lags were neglected.

Figure 58 presents six more data sets for the same substrate as shown in Figure 57. While the same general comments apply in Figure 58, data set #5C is anomalous in that M2 on page E-72 regresses negative values for both  $k$  and  $K$ --not just the latter. While it was stated in Section 6.1.2 that this happens when the data apparently drop at a greater-than-first-order rate, it also occurs if the overall trend in the data can be interpreted as  $S$  increasing with time (it is noted that  $S$  in reality cannot increase with time and that the observed trend is the result of random errors in the measurement of  $S$  during a period when biodegradation is not taking place). Because of the restriction of  $S_0$  equal to  $S(t=0)$  and because of the bulk of the data being in the lag phase where most of the  $S$  values are greater than  $S(t=0)$ , M2 regresses negative values of  $k$  and  $K$  to fit the observed data. Figure 17 graphically shows the predicted  $S$  vs  $t$  curve for a data set in which M3 regressed negative values of both  $k$  and  $K$  to fit an apparent greater-than-first-order drop. Figure 17 shows that two potential  $S$  vs  $t$  curves exist for positive values of  $t$ . It is the upper portion of the curve which accounts for the minimization of  $\Sigma(t-t_{calc})^2$  by the M2 model on page E-72 to result in negative values of  $k$  and  $K$ . Relaxation of the restriction of  $S_0$  equal to  $S(t=0)$  by the M3 model allows it to regress a positive value of  $k$  (but not  $K$  because of the apparent downward bend in the data set) in this case because of its interpretation of  $S$  in the data set as decreasing with time at less than a first-order rate.

Figure 59 shows four data sets (for nitrobenzene as substrate) which have a significantly shorter lag relative to the overall biodegradation time. As a result, the models evaluated in this thesis are better able to approximate complete data sets. Data sets #4B and #9B can be reasonably well-represented by F2 which just averages the error in the lag. M2 and M3 yield negative values of  $k$  and  $K$  for #4B, unlike positive values for #9B, because of the drop in #4B being greater-than-first-order. MV can (with accurate values of  $B_0$  and  $Y_c$ ) fit the data in #4B very well, but it also yields negative values of  $k$  and  $K$  for the same reason as M2 and M3. It is apparent from data sets #4B and #9B that a lack of data in the initial portions of the curves makes it difficult to be sure whether lags, or variable-biomass effects, or just random scatter in the data points are present. It is, therefore, imperative that biodegradation studies in batch reactors involve sampling at frequent enough intervals, and involve analyses of sufficient enough accuracy, to clearly define the initial lag region, and the transition from lag to utilization.

Figure 60 presents six data sets for N-nitrosodiethanolamine substrate as measured by Yordy and Alexander. The authors' sole premise was to assess the biodegradability of the specific substrate in various environments. They did not report analytical accuracy nor biomass measurements, nor did they perform any kinetic analyses. The very limited information as to the definition of the system makes the data of little practical value for design purposes.



Figures 61-63 present 15 data sets from three different sources yielding diverse results. Data set #8B in Figure 62 presents another example of M2 yielding negative values of both  $k$  and  $K$  for data which is not dropping at a greater-than-first-order rate (data set #5C in Figure 58 is the other example).

Figures 64-66 present 8 data sets from a total of 5 different literature sources. Figure 64 shows two data sets for the same system as shown in Figure 35 (refer to section 6.1.4). The length of the lag for this system is observed to increase with  $S_0$ , accounting for Klecka and Maier using the Haldane (substrate-inhibition) form of the Monod expression to model this entire system. Figure 65 presents three data sets from Papanastasiou and Maier which exhibit longer lags than another set from the same study which was previously discussed in Section 6.1.4 (refer to Figure 45). Papanastasiou and Maier used Andrews (substrate-inhibition) model to fit the data for 2,4-D and the MV model for glucose. For the case of glucose, MV can only provide a reasonable fit if the lag is neglected. The authors did not report  $Y_c$  and  $B_0$  for the glucose sets and, hence, comparison with their regressed results could not be facilitated.

Figure 65 also presents a data set from Liu, et al. The authors eliminated abiotic effects from the data via the use of a control, and determined a first-order rate constant (using least-squares analysis) after omitting those points in the acclimation phase. Data set #3 in Figure 65, however, is clearly seen to be of biodegradation type 6 (i.e., ZV) upon excluding the lag portion; the first-order model assumed by Liu, et al, is totally inappropriate for this set.

Figure 66 shows the last two data sets of type 7. The model shown for the data set from Saeger and Tucker is a second-order model (with the lag excluded). The lack of points in the initial region, combined with apparent scatter in the data, makes it difficult to be sure whether a lag truly exists. While the authors corrected the data for the abiotic substrate-removal mechanisms of chemical oxidation and volatilization, their control involved a sterile environment which did not assess whether adsorption onto biomass was significant. The greater-than-first-order drop observed may be due to the combined effects of adsorption and biodegradation.

The data set in Figure 66 from Shamat and Maier is best represented by the ZV model (with the lag excluded). The authors regressed the data (with the lag portion excluded) to the MV model to yield a  $\mu_m$  of  $0.05 \text{ day}^{-1}$  and a K of 25.3 ppm. The regressed results for the MV model on page D-73 are in reasonable agreement (i.e.,  $\mu_m = k_o/Y_c = 0.04 \text{ day}^{-1}$  and  $K = 20.6 \text{ ppm}$ ) considering the following

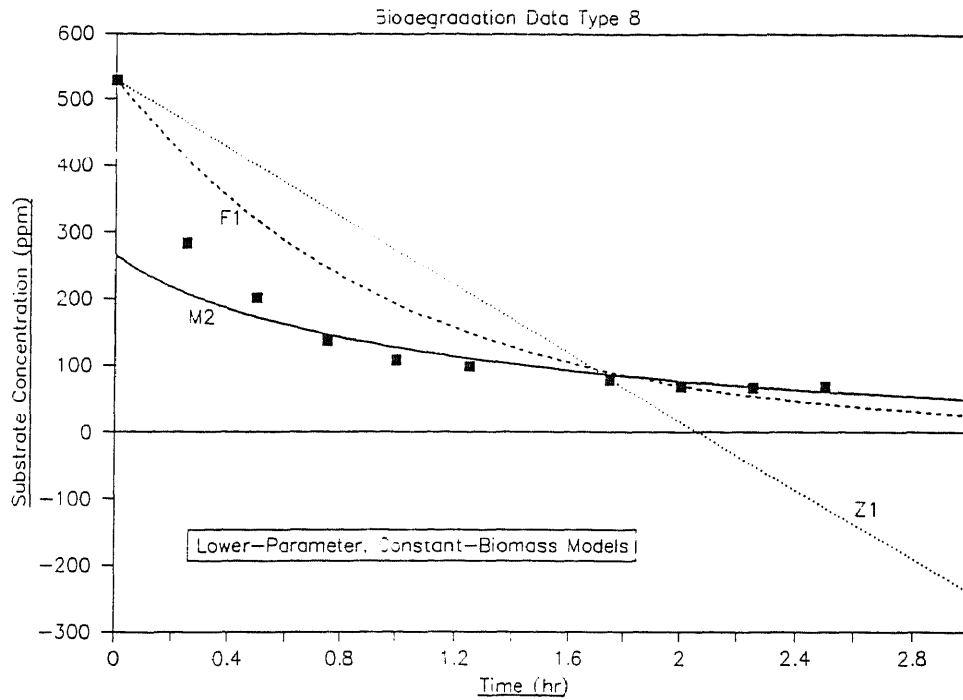
differences between the two sets of analyses: (1) the lag was included in the latter analysis accounting for the slightly lower value of  $\mu_m$ , and (2) the authors did not report the value of  $Y_c$ , requiring an estimated value (based on comparable substrate  $Y_c$  values reported by them) to be used.

#### 6.1.8 Data Type 8 (Greater-Than-First-Order Drop)

This biodegradation data type refers to those data sets which exhibit a definitively greater-than-first-order drop. This may be due to the simultaneous action of multiple substrate-elimination mechanisms (e.g., abiotic mechanisms, such as adsorption, volatilization and chemical oxidation), and not just biodegradation. Biodegradation of nth-order kinetics greater than one is not common. Therefore, description of this type of data as a separate "biodegradation" type in the pure sense of the term may not be correct. However, it is grouped and discussed separately here because of its occurrence in the literature, and the need to address concerns with respect to the modelling and utilization of these data for design purposes.

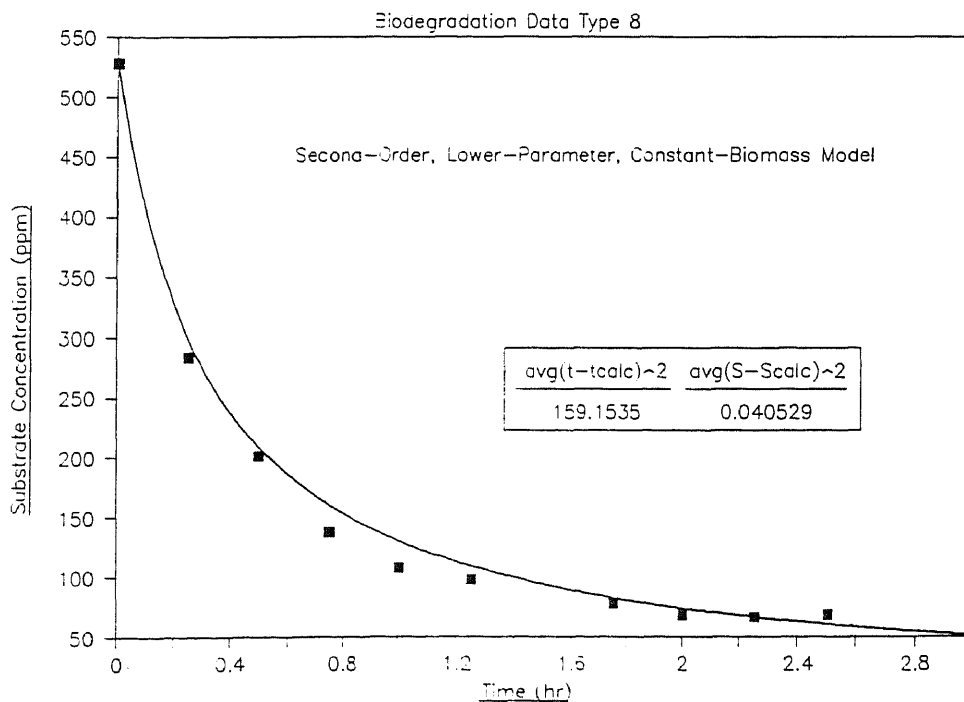
Figure 67 presents a data set measured by Chudoba, et al, which is of biodegradation data type 8. The constant-biomass models evaluated in this thesis on page D-24 are inappropriate for this specific case, as well as for this data type in general (refer to Figure 67 for a visual presentation of the Z1, F1 and M2 models). The Monod models are statistically best of those evaluated, but regress negative values of both

Figure 67



Source: Chudoba, J., Grau, P. & Ottova, V. (data set #1 shown on page D-24)

Figure 68



Source: Chudoba, J., Grau, P. & Ottova, V. (data set #1 shown on page D-24)

k and K for data of greater-than-first order (as mentioned previously in Section 6.1.2). Even with the negative rate constants, however, the Monod models are incapable of fitting data much greater in order than first. While the zero- and first-order models always regress positive rate constants, they are both worse in terms of fit than the Monod with the zero-order being incapable of modelling any curvature and the first-order underestimating the rate of drop.

Chudoba, et al, used a second-order model (as shown in Figure 68) to fit the data set shown in Figure 67. This data set is different from all the others evaluated in this thesis in that it is for more than one substrate (i.e., peptone and starch) with S being quantitated in terms of COD. Grau and Dohanyos<sup>6</sup>, on the basis of numerous experiments and thorough theoretical analysis, proposed the following differential equation for multicomponent substrate-removal kinetics:

$$-dS/dt = k_n B_o (S/S_o)^n \quad ; \quad (3)$$

where,

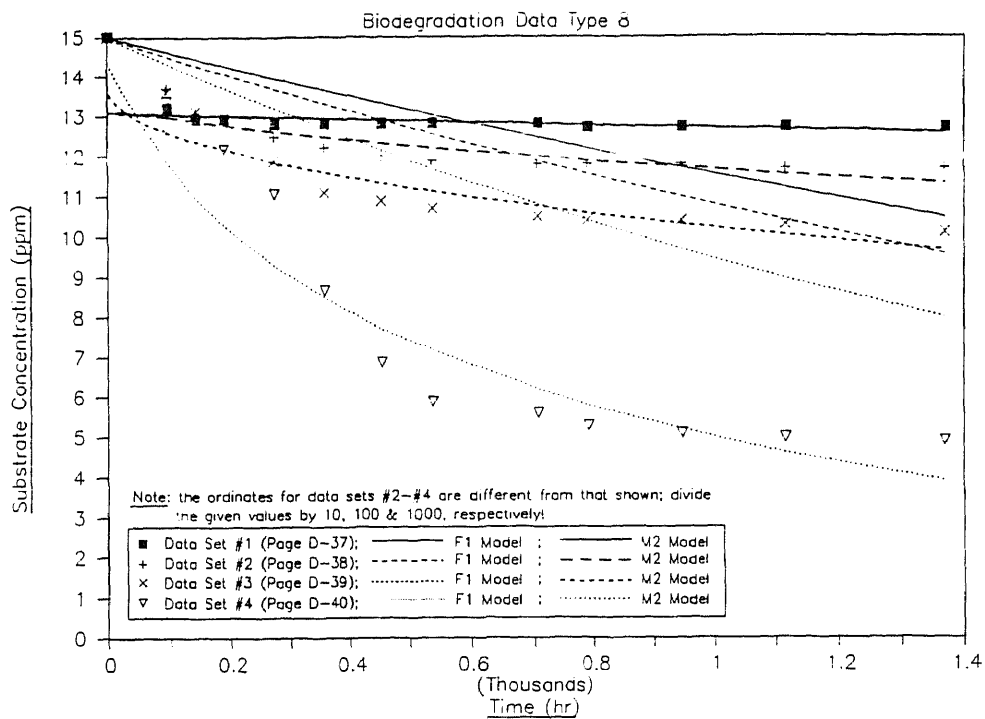
$k_n$  = specific substrate-removal rate constant of the nth order.

$n$  = formal order of the reaction.

Equation (3) applies when the microorganisms do not compete for the same substrate. It is uncertain as to whether the previous assumption is correct for this data set or whether other, unaccounted-for, abiotic removal mechanisms are responsible for the greater-than-first-order drop observed in the data since no mention was made by the authors as to the magnitude of the abiotic effects.

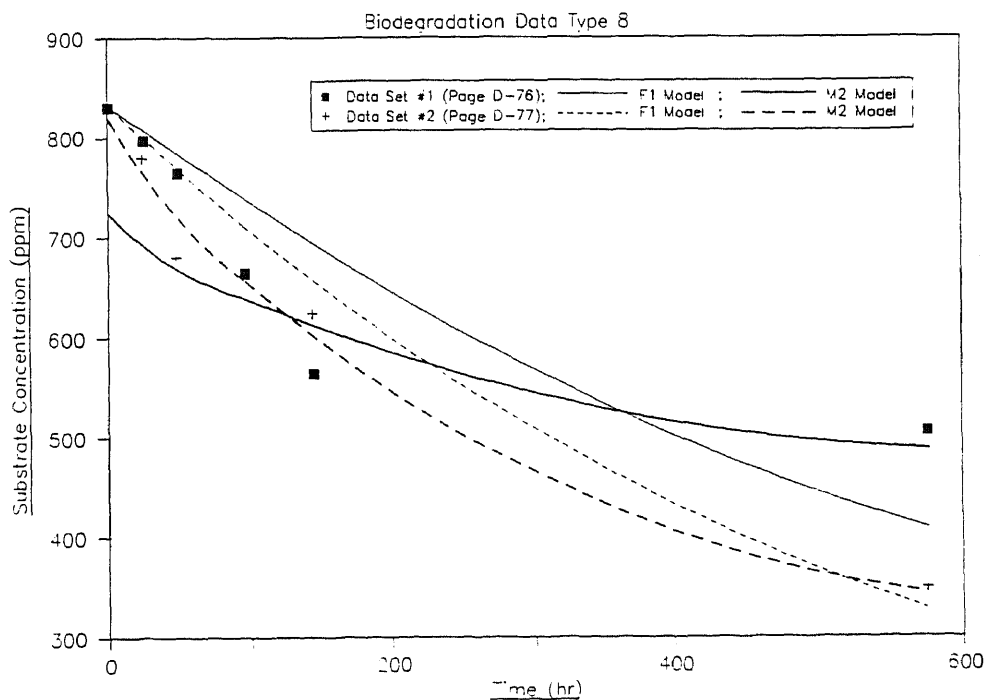
In addition to the data set shown in Figures 67 and 68, 13 more of the 124 mixed-culture data sets evaluated in this thesis are categorized as data type 8. These sets are all presented graphically in Figures 69-74 along with the corresponding F1 and M2 curves. All of these sets have the common characteristic of regressing negative values of both  $k$  and  $K$  for the Monod models (i.e., M2 and M3). Unlike the previously discussed data set, these sets are for single-substrate systems where the  $n$ th-order model presented as Equation (3) is not applicable. No generally-accepted kinetic theory is currently available to support the observed cases of  $n$ th-order biodegradation of greater-than-first order. The observed greater-than-first-order kinetics are regarded as artifacts of the data which may be attributed to any, or all of the following: (1) inaccurate measurements, (2) unaccounted-for, abiotic, substrate-removal mechanisms, (3) product inhibition resulting in a dramatic decrease in substrate-utilization rate which, in turn, results in the data set being interpreted as type 8, and (4) some other essential nutrient becomes limiting instead of the substrate which would have a similar effect to that of product inhibition.

Figure 69

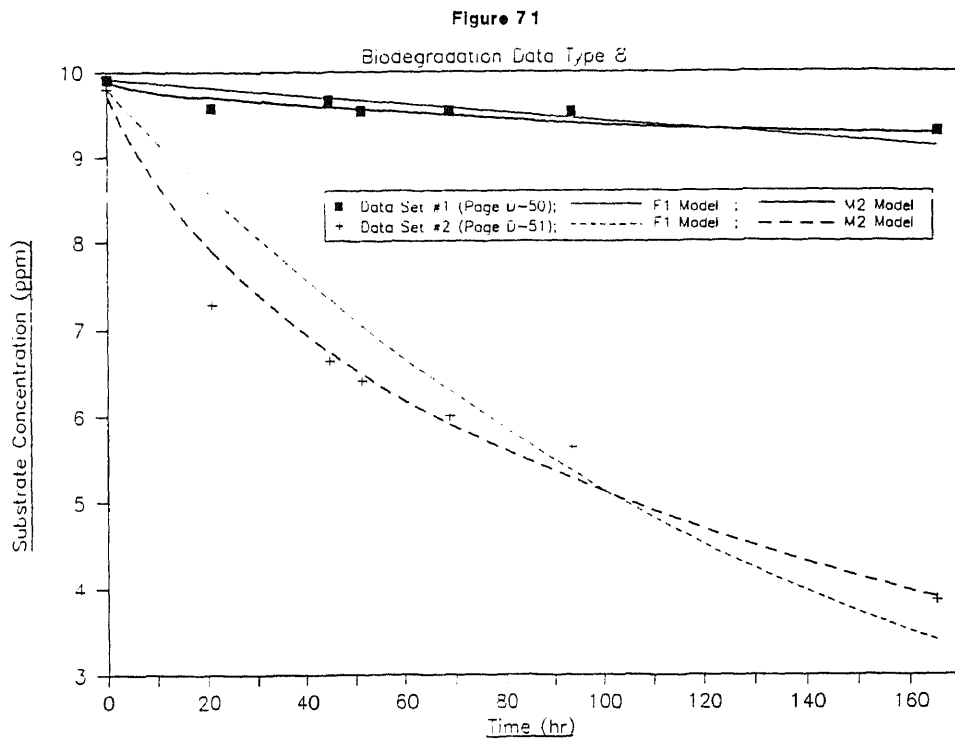


Source: Kaplan, D.L. & Kaplan, A.M. (data sets #1-4 shown on pages D-37 to 40)

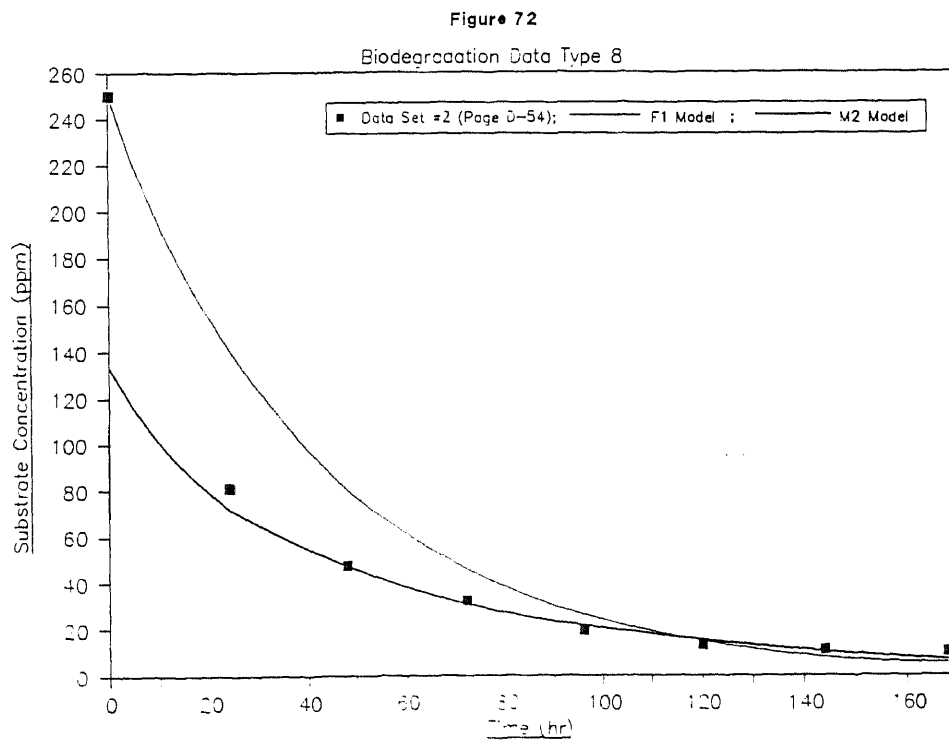
Figure 70



Source: Taylor, B.F. & Ribbons, D.W. (data sets #1 & #2 shown on pages D-76/7)



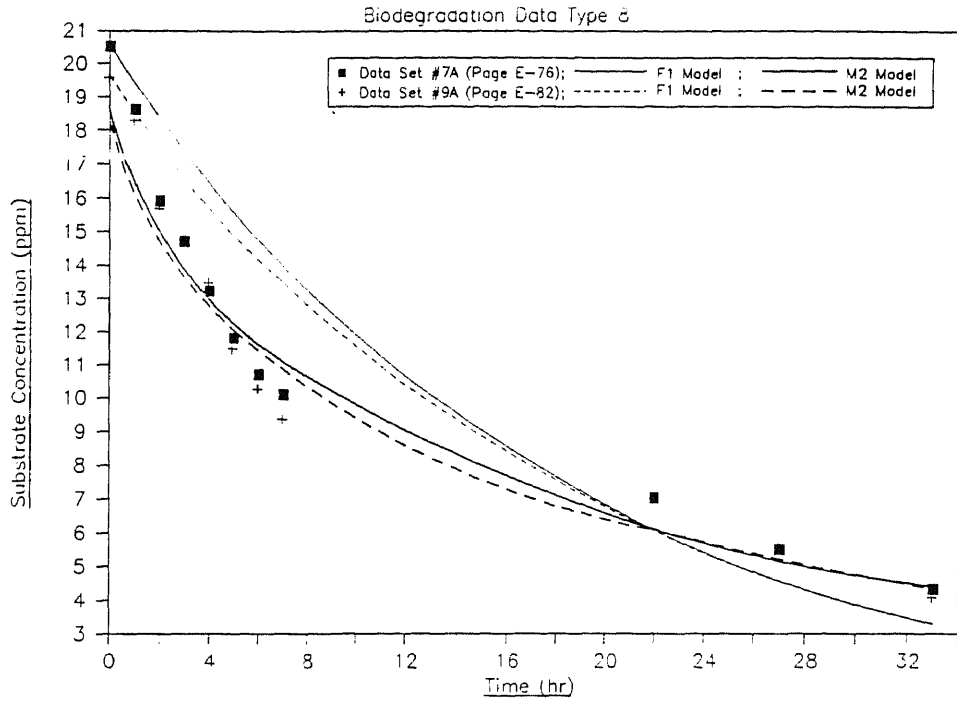
Source : Liu, D., et al (data sets #1 & #2 shown on pages D-50 & D-51)



Source : Lyons, C.D., Katz, S. & Bartha, R.

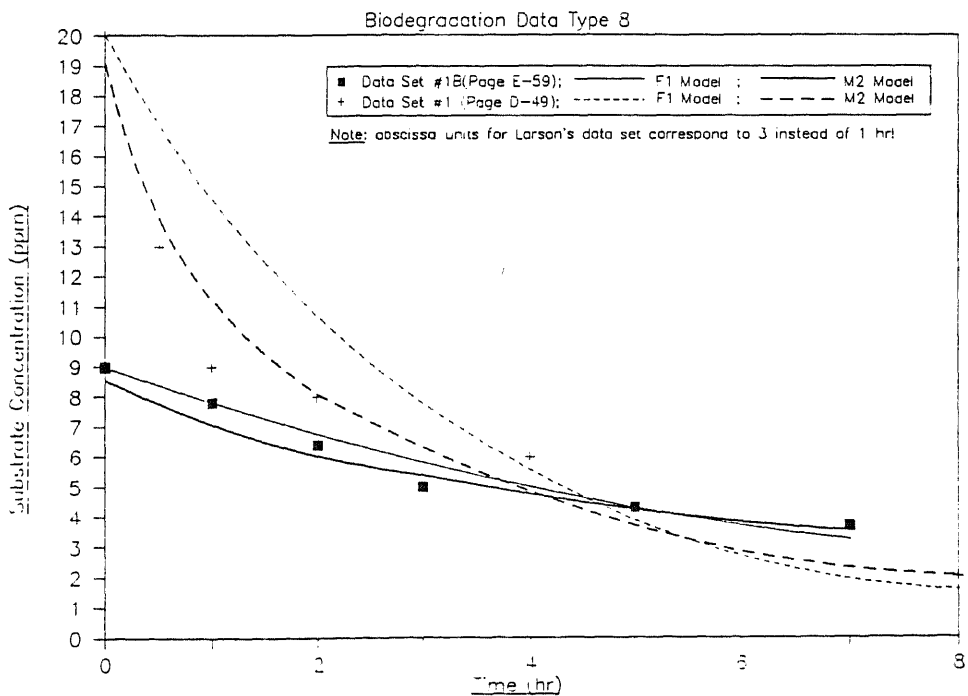


Figure 73



Source : Naik Thesis (data sets #7A & #9A shown on pages E-76 & E-82)

Figure 74



■ Source : Naik Thesis (data set #1B on page E-59)  
 + Source : Larson, R.J., Games, L.M. & King, J.E. (data set #1 on page D-49)

Figure 69 presents four data sets from Kaplan and Kaplan which are of type 8 primarily because of inaccuracies in the method which the authors used to determine S. Instead of measuring S directly, they radioactively labelled the substrate and quantitated the rate of biodegradation by detecting  $^{14}\text{C}$  in traps as a function of time. Their questionable assumptions of biodegradation leading to complete mineralization (i.e., without any assimilation), and of the traps being 100% efficient, were not validated. The errors caused by these inaccurate assumptions in the back-calculated S vs t data likely account for the observed S levelling off at values higher than actual. Furthermore, the authors did not assess whether abiotic effects or product inhibition were contributing factors. It should be noted that the authors did evaluate Michaelis-Menten kinetics following manipulation of these data sets. They estimated the instantaneous reaction rate for each set and then regressed the obtained values vs. S for each set. They found the data to be first order with  $K \gg S$ . Whereas the authors reduced the errors in their kinetic analysis via the data manipulation, the validity of the results obtained are no less questionable as abiotic effects were not addressed.

Figure 70 presents the data sets from Taylor and Ribbons. Both are interpreted as type 8 largely because of the last point in each being high. The missing points in the intermediate region of each set along with apparent data inaccuracy make these sets of no practical value from a kinetic analysis perspective.

Figure 71 presents two data sets from Liu, et al, for which the authors subtracted contributions due to abiotic effects based on control runs. While significant data scatter is present in both sets, it is apparent that  $S$  drops at a greater-than-first-order rate. The authors, however, erroneously regressed these data to first-order models (as they also did for a set shown in Figure 65 and discussed in Section 6.1.7 on page 106). They regressed first-order rate constants of 0.0004/hr and 0.0053/hr for data sets #1 and #2, respectively. Based on a comparison with the corresponding regression results shown on pages D-50 and D-51, it appears that the authors used the F2 version of the first-order model for their analyses.

The data set shown in Figure 72 from Lyons, et al, is not corrected for the effect of abiotic mechanisms although the authors did attempt to assess the relative contributions of evaporation, auto-oxidation and adsorption. Even after correcting the data for the above-mentioned abiotic effects, however, the set is still clearly greater than first order. The authors' techniques for quantification of abiotic effects were not validated, and it is possible that the adsorption effect, as a result, was underestimated. The other data set from this literature source was categorized as type 2 (refer to Figure 21 in Section 6.1.2). The system used for this data set had a much lower level of biomass (i.e., pond water vs sludge) which would account for the contribution of the adsorption effect being significantly reduced in its case.



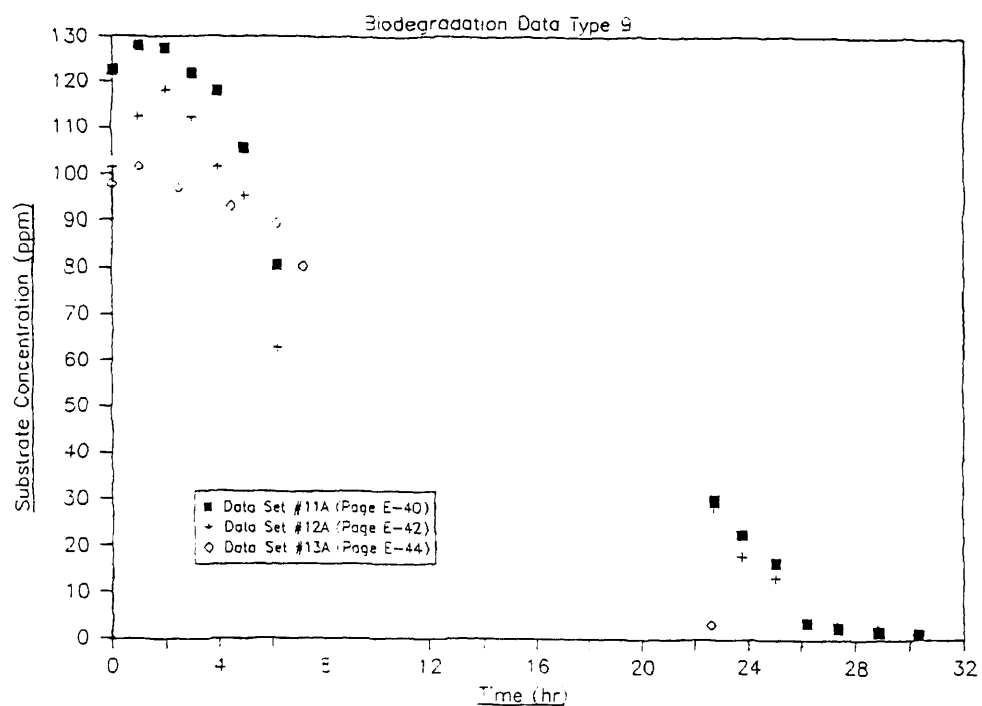
It should be noted here that the variable-biomass models are capable of fitting greater-than-first-order kinetics with positive rate constants when negative yield constants are used. This was briefly discussed in Section 6.1.4 (refer to Figures 40, 42 and 44). Negative values of  $Y_c$ , however, while potentially possible (i.e., during periods of net cell death), are not the norm.

#### 6.1.9 Data Type 9 (Miscellaneous)

The remaining 12 data sets for batch-reactor, mixed-culture systems (not previously discussed in Sections 6.1.1 through 6.1.8) are covered in this section under the broad category of miscellaneous. These sets are classified as type 9 for the most part because of their poor quality data (e.g., high scatter, missing points and/or apparently erroneous measurements). As a result, the data sets are either different from types 1-8, or intermediate between two or more types, with selection of the correct one not being able to be made conclusively.

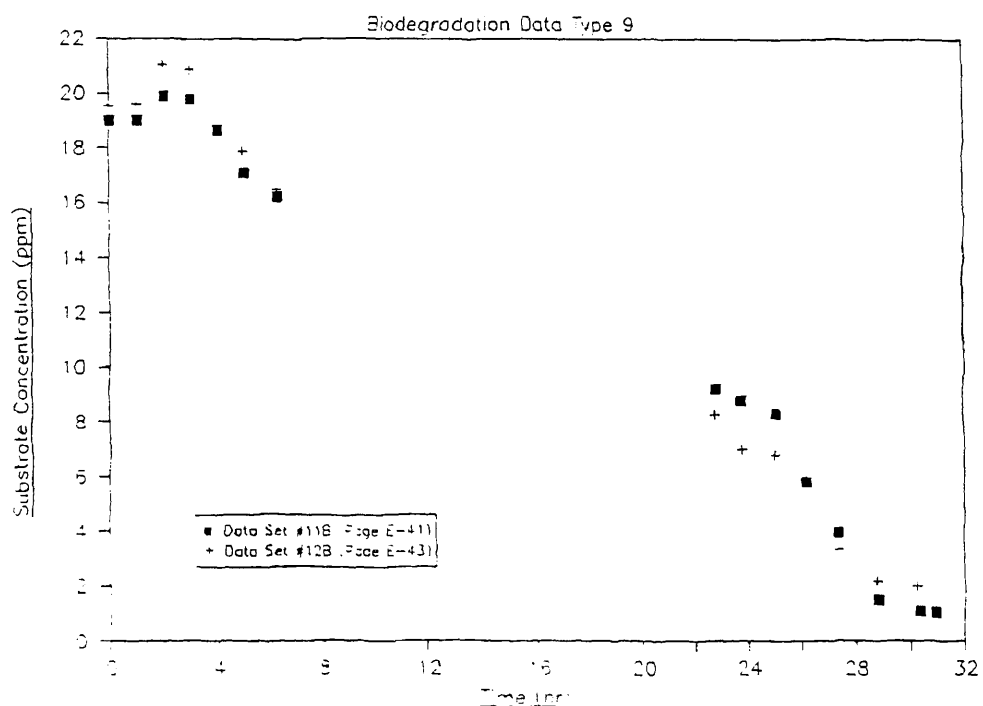
Figures 75 and 76 present 5 data sets from the Gonnabathula thesis which are of type 9 because of the very poor quality of the data. The combination of high data scatter and omission of data points in the central (i.e., overnight) time period makes selection of the specific data type impossible. Kinetic analysis of these sets yields little of practical value. The only

Figure 75



Source : Gonnabathula Thesis (phenol as substrate in mlss)

Figure 76



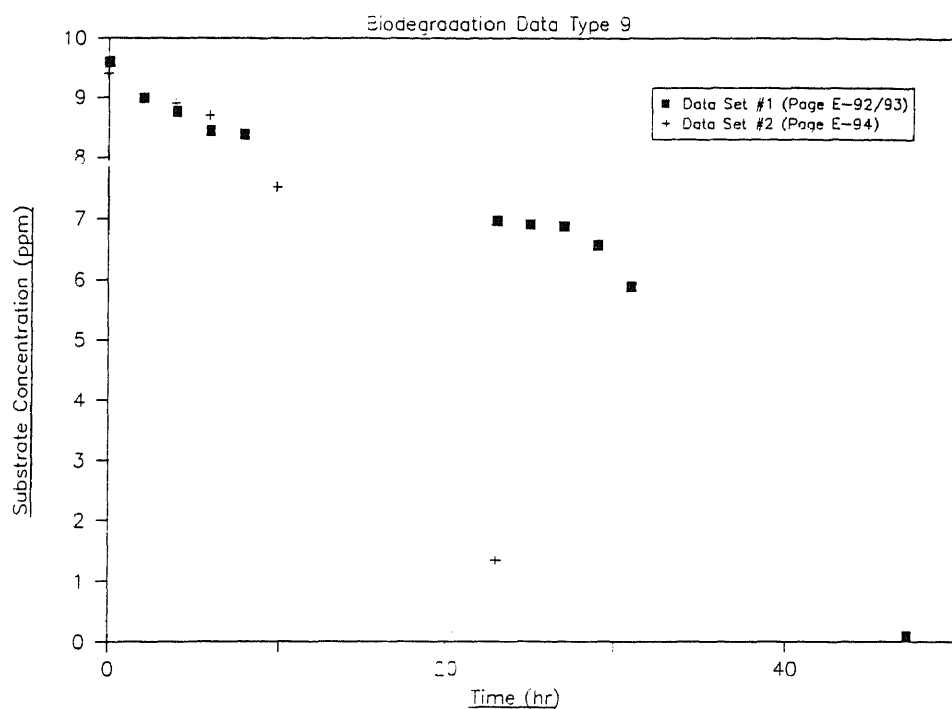
Source : Gonnabathula Thesis (nitrobenzene as substrate in mlss)

information of value to be deduced from these sets is that: (1) lags are present, and (2) biodegradation down to certain levels takes place within given time periods. Knowledge of the  $S$  vs  $t$  profiles, however, cannot with any reliability be predicted from these data.

Figure 77 graphically presents 2 data sets from Pak's thesis which show slow but steady degradation prior to the last point of each set. The last point of each set is much lower than expected which may be due to either some unexplained change in the culture which results in a dramatic increase in its activity or it may just be an artifact of the analytical method. Without data from the intermediate, overnight periods, however, the true nature of these sets cannot be determined.

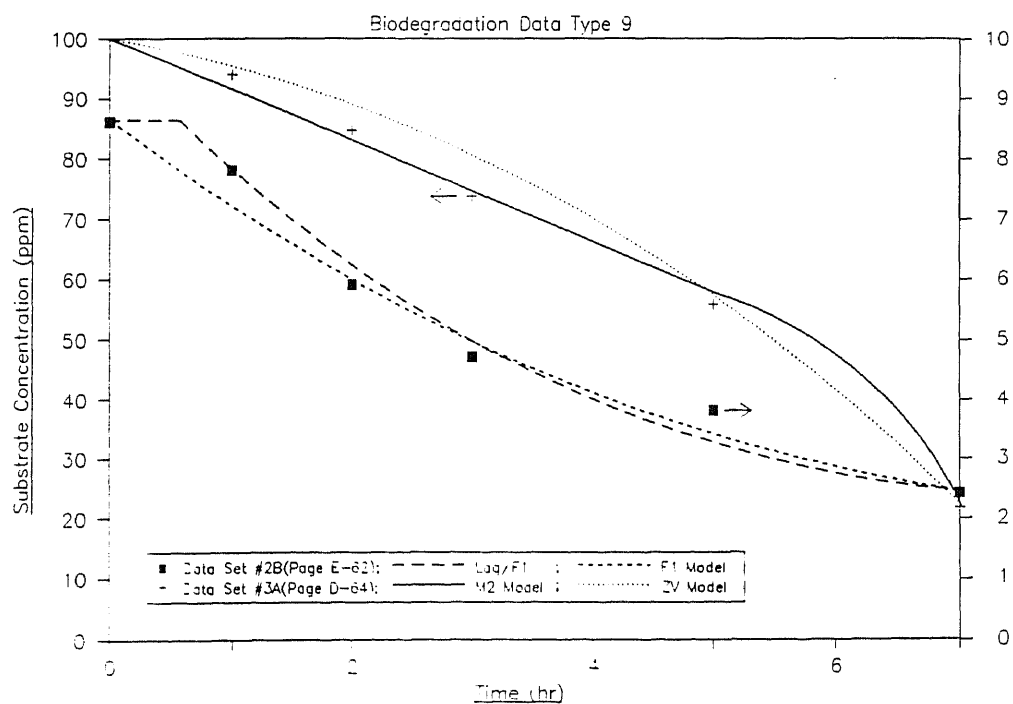
Figure 78 shows 2 data sets from the Naik thesis which are of better quality than the preceding sets in this section. Data set #2B exhibits sufficient scatter, however, to make conclusive interpretation of its specific data type difficult (e.g., it can be any of types 2,3,4,5,7 or 8). Figure 78 shows the F1 model with and without lag for comparison purposes. Data set #3A is shown to be very well represented by the M2 model with a negative value of  $K$  (because of the apparent downward bend in the data). Whereas the ZV model can fit a downward bend with a positive rate constant, it is incapable of fitting a shape like this, with a linear drop followed by a sudden

Figure 77



Source : Pak Thesis (2,6-dichlorophenol in activated sludge)

Figure 78



Source : Naik Thesis (substrates in unacclimated sludge)

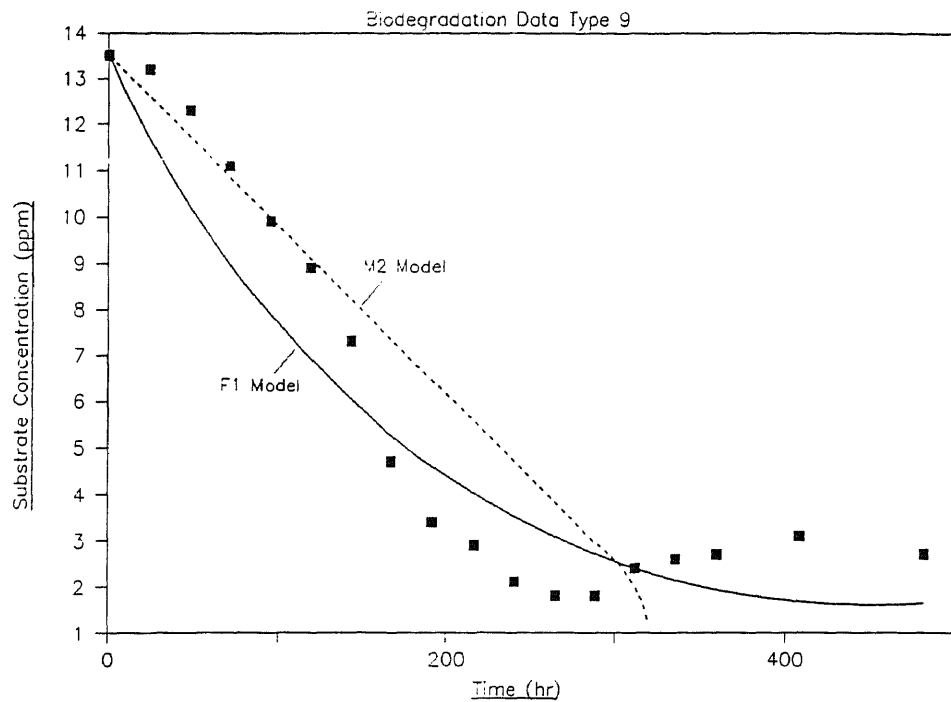


increase in the biodegradation rate. A hypothetical ZV model is provided in Figure 78 for comparison purposes ( $B_0$  was selected for an assumed  $Y_c$  of 0.5 so as to minimize  $\Sigma(t-t_{calc})^2$ ). Additional data points in the latter region of this set would have provided more information with which to better interpret its kinetics. As presented, however, the integrity of the last data point is questioned.

Figure 79 presents a data set from Blanchard, et al, which appears to demonstrate MV kinetics in the initial half of the set. The second half of the set exhibits the anomalous effect of  $S$  increasing with  $t$ , which is likely an artifact of the authors' analytical procedure. The authors radioactively labelled the methylcellulose substrate, then measured the radioactivity in the supernatant as a function of time, and related the detected  $^{14}\text{C}$ -concentration to  $S$ . The observed apparent increase in  $S$  may have been the result of the release of  $^{14}\text{C}$  into the supernatant as part of soluble by-products of endogenous respiration. Blanchard, et al, summarized the results of their experiment with a zero-order rate constant to represent the rate of substrate utilization. Representation of the data as zero-order is a poor approximation, but the apparent inaccuracy of the data negates the practical utility of an accurate kinetic analysis.

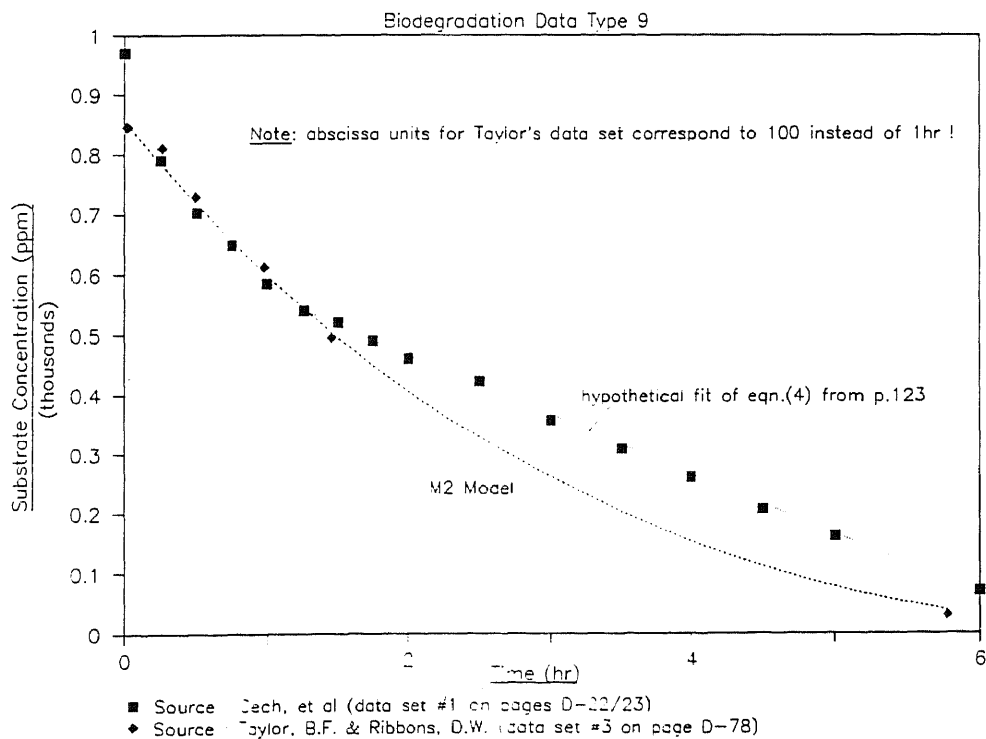
The remaining 2 data sets categorized under type 9 are presented in Figure 80. The set from Cech, et al, is unusual in that the initial drop is rapid and of first-order nature before transition to a slower, zero-order drop. The authors attributed the

Figure 79



Source : Blanchard, et al (refer to data set #1 on pages D-20/21)

Figure 80



initial rapid drop to the accumulation capacity of the involved microorganisms for the substrate. They used the following model based on storage and accumulation processes to represent the data:

$$-dS/dt = K_0 + K_1 S_{ra} \exp(-K_1 t); \quad (4)$$

where,

$K_0$  = zero-order rate constant due to storing processes

$K_1$  = first-order rate constant due to accumulation processes

$S_{ra}$  = apparent volumetric accumulation capacity

Equation (4) may be a suitable approach for modelling the combined effects of biodegradation and adsorption simultaneously. The models on pages D-22 and D-23 show MV to yield negative values of  $k$  and  $K$  while M2 and M3 yield positive rate constants. The MV model would have yielded positive rate constants if a negative value of  $Y_c$  were used.

The data set in Figure 80 from Taylor and Ribbons is well represented by the Monod model (i.e., type 3) but appears to exhibit a possible lag based on the second data point being higher than predicted, which would result in this set being classified as type 7. Lack of data in the initial portion of this set makes conclusive categorization difficult. Based on the relatively small magnitude of the alleged lag relative to the overall biodegradation

time frame, however, it has little practical impact on the fitting of the data unless interest lies specifically with the initial portion of the data set. It should be noted that the two other data sets from Taylor and Ribbons were categorized as type 8 (refer to Figure 70). The lack of data points in the region preceding the last point of each set places too much reliance from the kinetic analysis perspective on the integrity of the last point of each set. Whereas data sets #1 and #2 were interpreted as greater-than-first order and data set #3 as less-than-first order, the interpretation by the models is determined by the accuracy of the last point of each set and may just be the result of experimental error and not necessarily reality.

## 6.2 Batch Reactor Data--Single Culture Systems

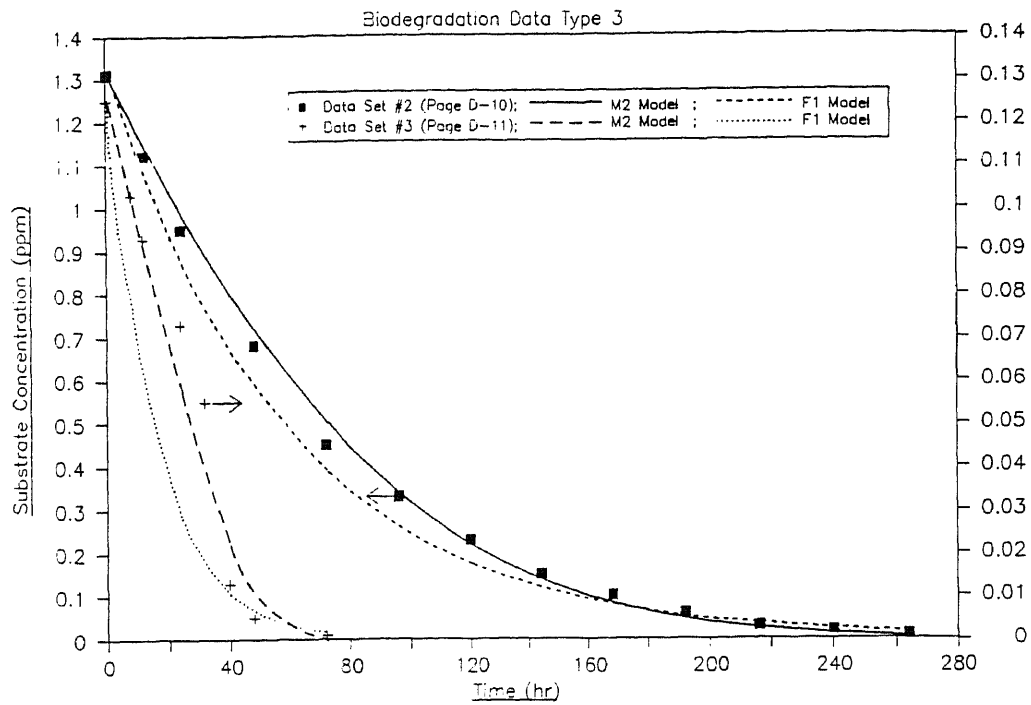
Whereas the bulk of the batch reactor data sets evaluated in this thesis are for mixed-culture systems, a significant proportion of those extracted from the literature (i.e., 16 of 54) involved single-culture systems. While single-culture systems are not common in industrial wastewater treatment operations, nor in natural environments, certain species may dominate the response of a heterogeneous population (e.g., activated sludge) to a give substrate. Study of single-culture systems usually results in more reliable kinetic data than mixed-culture systems (providing abiotic substrate-removal mechanisms are accounted for) because: (1) the active biomass concentration can be more readily determined; and (2) there is no shift in population during the course of an experimental run. A higher proportion of the bacteria are active

in substrate-specific, single-culture systems than in mixed-culture systems. Measurement of kinetic data, however, should be performed at relatively high food-to-microorganism ratios (i.e., S/B) to avoid conditions of endogenous respiration where the percentage of active biomass is noted to decrease substantially.

The discussion of all of the data sets for single-culture systems will be conducted within this section as the total number is tractable and the characteristics of each individual data type (specifically with respect to modelling by the constant- and variable-biomass versions of the zero-order, first-order and Monod kinetic models) were already covered in detail in Sections 6.1.1 through 6.1.9.

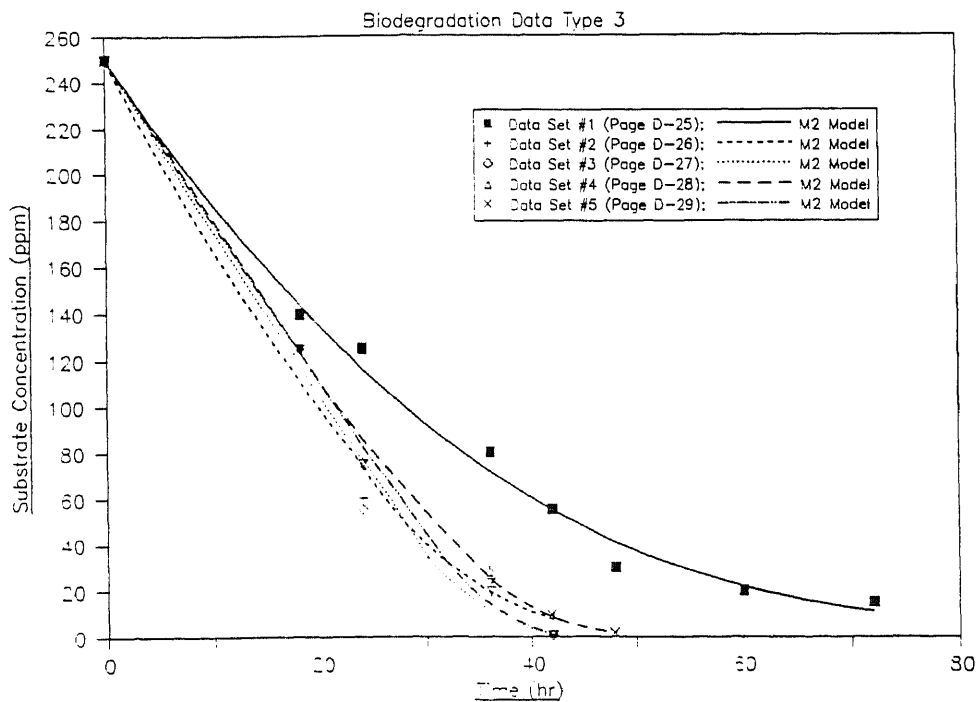
The bulk of the single-culture systems investigated in this thesis (i.e., 9 of 16) are categorized as biodegradation data type 3. Figure 81 presents 2 of these data sets which were extracted from an article by Allard, et al. The M2 models are shown to well represent both cases; the corresponding F1 models are presented for comparison purposes and clearly show the reaction order in each case to be less than one. The increased scatter in data set #3 vs #2 is the result of decreased analytical accuracy at lower S values. The objective of the study by Allard, et al, was to assess the impact of discharges of chloroguaiacols into the environment. Even though the authors noted the data sets to be concentration dependent, they estimated pseudo-zero order rate constants from linear portions of the curves and converted

Figure 81



Source : Allard, A.S., et al (3,4,5-trichloroguaiacol in strain 1395)

Figure 82



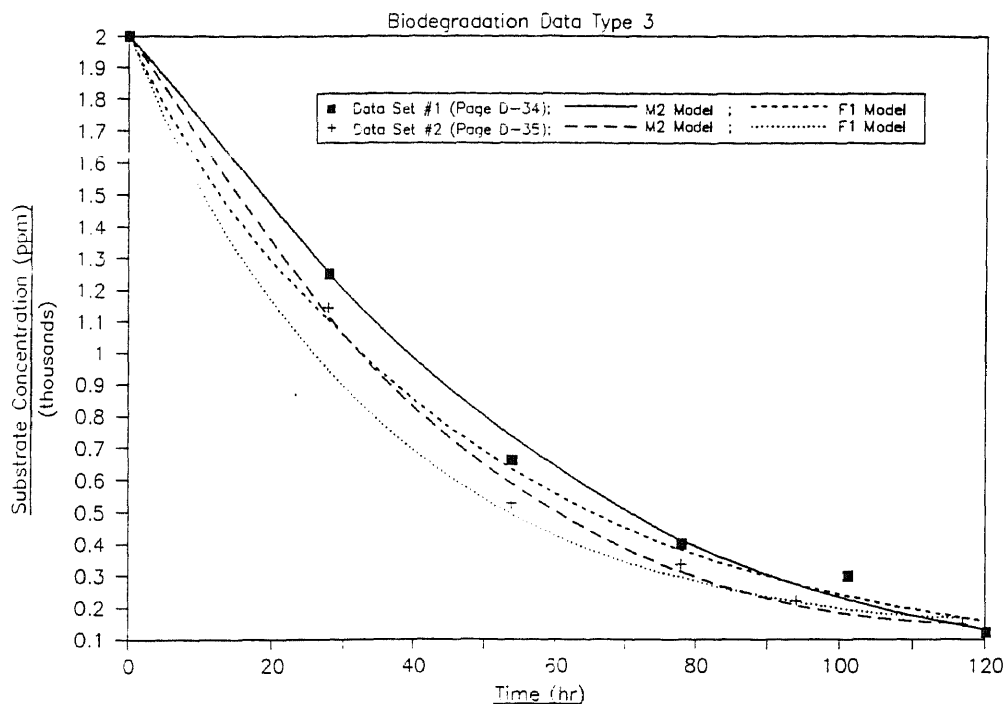
Source : Garbarr, S.V. & Rotmistrov, M.N. (HMDA in B.subtilis)

them into specific rates by dividing by the cell density. The variable-biomass models were not evaluated in Appendix D for these 2 sets for the following reasons: (1) adequate biomass data were not presented by the authors, (2) no variable-biomass effect was evident in the data sets, and (3) the authors classified the biomass as non-proliferating and stated that  $B$  was virtually constant throughout both experiments. The authors also noted difficulty in obtaining accurate biomass measurements due to problems with plating the dense cultures which were used.

Figure 82 presents 5 data sets of type 3 from Garbara and Rotmistrov which are well represented by the M2 models. The article's primary purpose was to study the oxidative and degradative activity of B.subtilis, which utilizes hexamethylenediamine (HMDA) as the sole nitrogen and carbon source, and the effect of clay minerals on these processes. Biomass measurements were not presented by the authors nor were kinetic analyses performed.

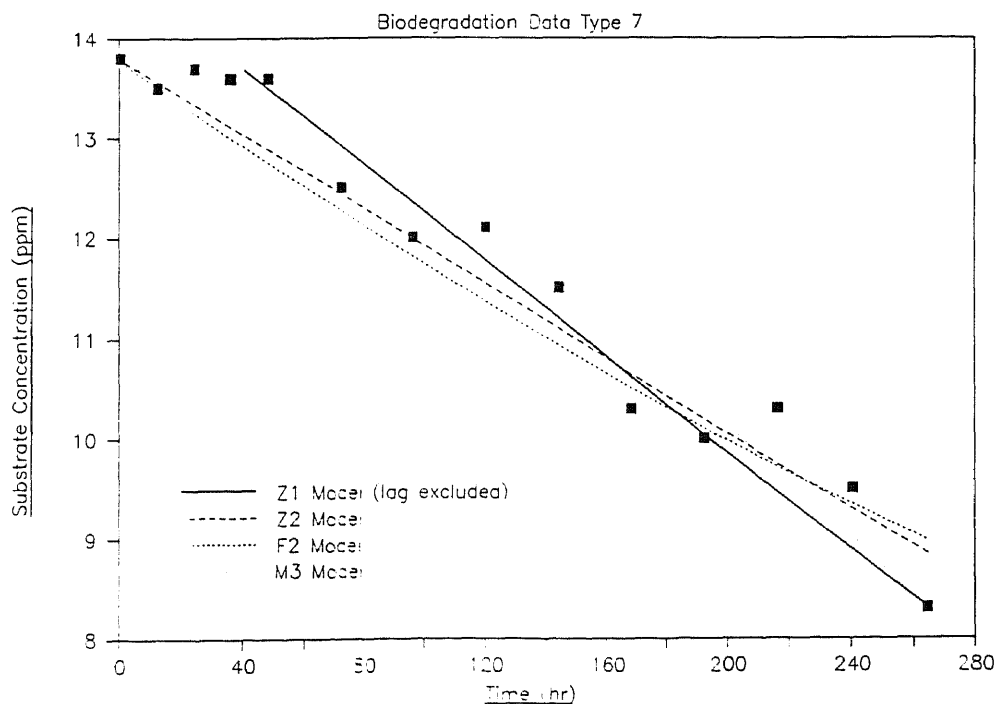
The remaining 2 single-culture data sets of type 3 were extracted from Ilyalendinov, et al, and are presented in Figure 83. Both sets are slightly less than first order and are shown to be well represented by the M2 models. Whereas variable-biomass data were provided by the authors for both cases,  $Y_c$  was far from constant indicating that the assumption of exponential growth throughout the  $S$  range covered was not valid; the variable-biomass models were, therefore, not valid and, hence, not evaluated. Data set #3 from

Figure 83



Source : Ilyalendinov, et al (alpha-methylstyrene as substrate)

Figure 84



Source : Allard, A.S., et al (refer to data set #1 on page D-9)

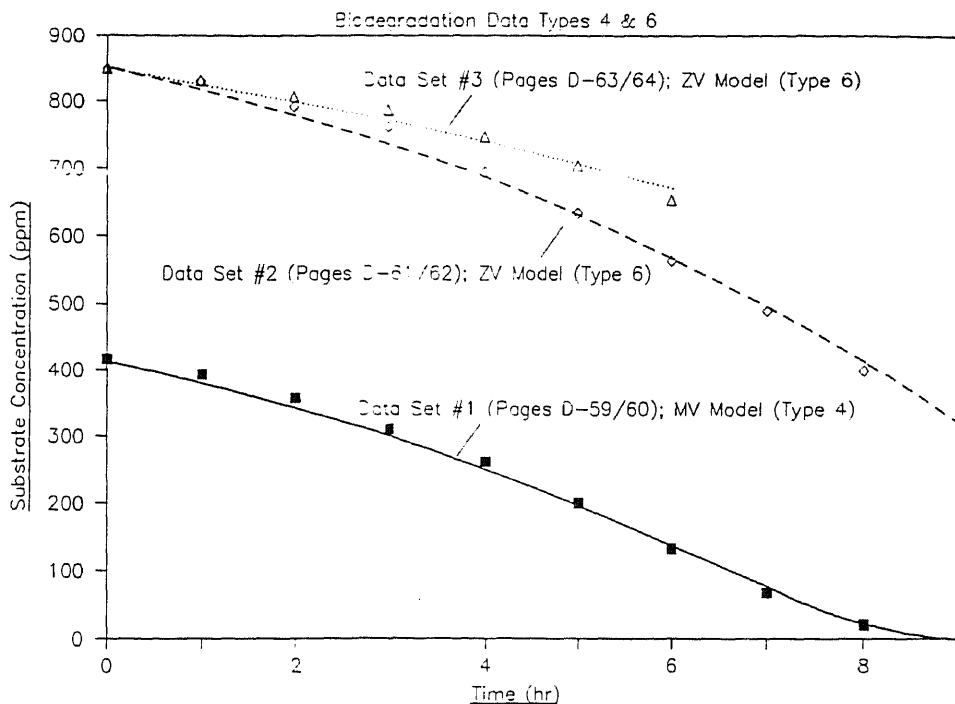


Ilyalendinov, et al, was classified as type 4 (refer to the figures on page 65); data sets #1 and #2 may also possibly be of type 4, but the lack of information available on the data sets (i.e., lack of points in the initial region, no report of analytical accuracy, and lack of reliable variable-biomass data) does not substantiate such a conclusion.

The other 7 of 16 single-culture data sets studied in this thesis are of types 4, 6 and 7. Figure 84 shows data set #1 from Allard, et al, to be of type 7. Because of the relatively high data scatter and the small S range covered (and because the lag is short relative to the overall biodegradation time), none of the models shown on page D-9 result in bad fits. While the Monod models are the best of those shown on page D-9, they both result in negative values of K due to the apparent downward bend in the S vs t data. Figure 84 visually shows the constant-biomass, zero-order model (with the lag excluded) to be the best for this data set.

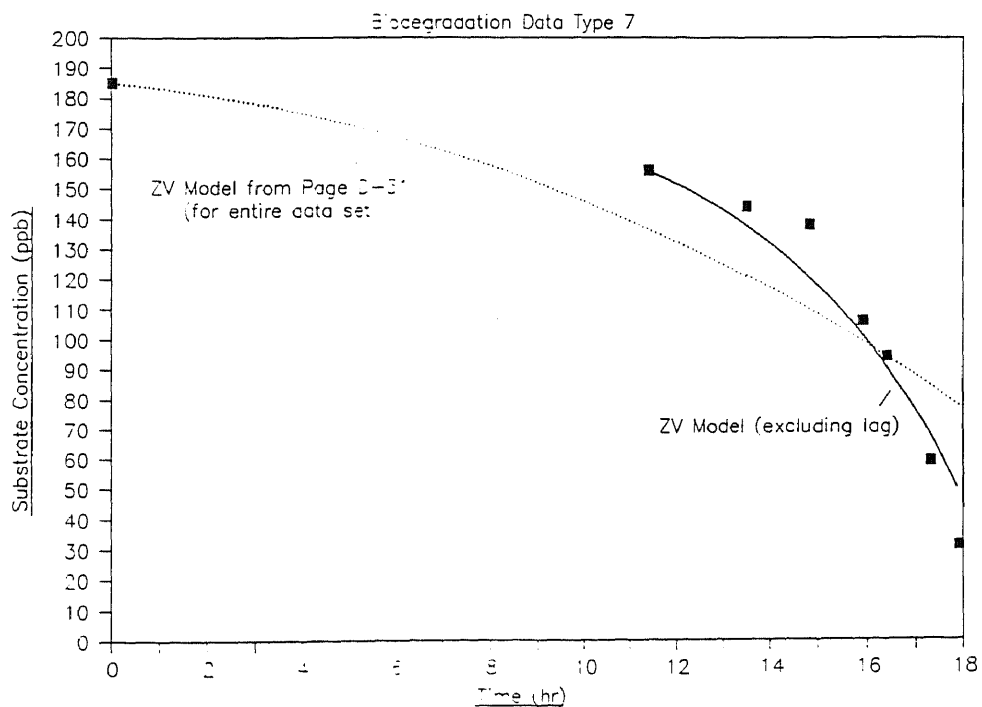
Figure 85 shows 3 data sets from Radhakrishnan and Sinha Ray (for phenol in B.cereus) to be well-represented by the variable-biomass models utilizing the biomass data measured by the authors using a Klett-Summerson photoelectric colorimeter. Data set #1 is of type 4 and is shown to be very well-represented by the MV model from page D-60; the measured values of  $B_0$  and  $Y_c$  result in a near optimum fit for the MV

Figure 85



Source : Radhakrishnan, S. & Sinha Ray, A.K. (phenol in *B.cereus*)

Figure 86



Source : Hill, G.A. & Robinson, J.W. (refer to data set #1 on pages D-30 & 31)

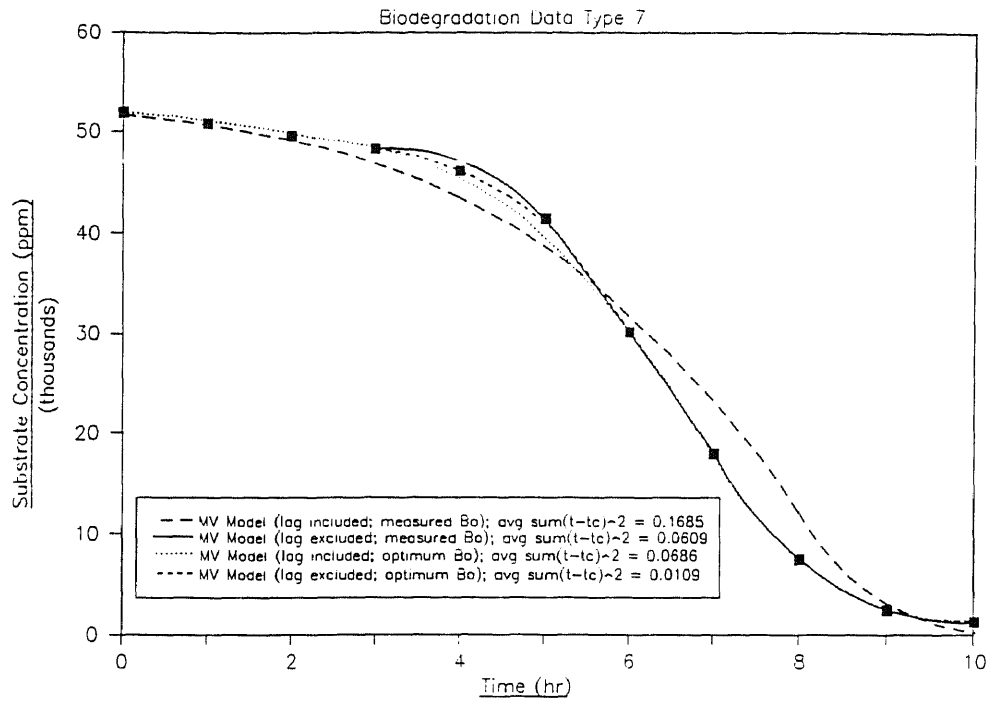
model. The predicted curve has a slightly smaller variable-biomass effect than actually observed which may be due to the measured  $B_0$  being slightly higher than the actual viable biomass concentration; this is likely since the photoelectric colorimeter measures the total (not active) biomass concentration. Data sets #2 and #3 are both of type 6 and are shown to be fairly well represented by the ZV models from pages D-62 and D-64, respectively. In each case, however, the measured value of  $B_0$  is higher than the actual active biomass concentration resulting in the variable-biomass models underpredicting the variable-biomass effects observed. The higher-than-actual  $B_0$  (active biomass concentration) values account for the MV models on pages D-62 and D-64 regressing negative values of  $K$  in order to best fit the data sets. For the values of  $Y_c$  used in data sets #2 and #3, the values of  $B_0$  would have to be less than 95 ppm and 40 ppm (instead of the measured values of 143 ppm and 155 ppm), respectively, for the MV models to regress positive values of  $K$ .

The remaining 3 single-culture data sets exhibit lags and are classified under the category of biodegradation data type 7. Figure 86 presents the first of the 3 which was extracted from an article by Hill and Robinson. Figure 86 shows the ZV model from page D-31 (which includes the lag portion in the regression analysis) and the corresponding ZV model for which the lag portion was excluded from the regression analysis. While better performance is apparent in the latter

case, both models underpredict the observed variable-biomass effect because of an overprediction of  $B_0$ , which is the result of the biomass measurement technique used (i.e., optical density) being a measure of the total, and not active, biomass concentration. It should be noted that the variable-biomass models are not theoretically valid for the data set shown on page D-31 since they assume that the biomass is in the exponential growth phase over the entire range considered, which is apparently not the case here (i.e., the lag is present). The authors excluded the lag from their kinetic analysis in which they studied the more complex substrate-inhibition models (e.g., Haldane, Andrews and Aiba-Edwards equations).

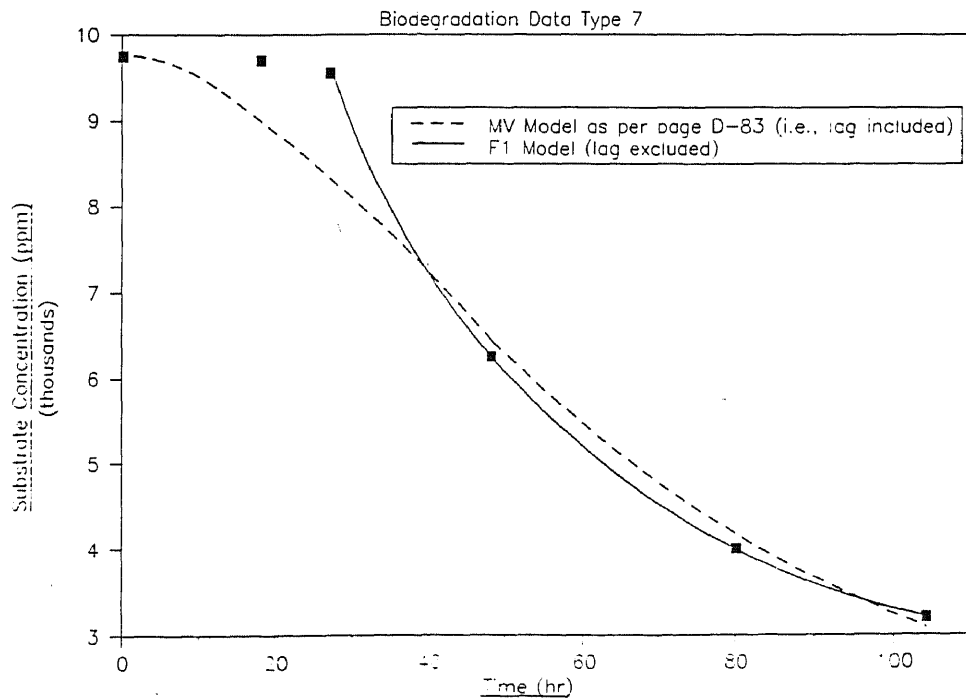
The second single-culture data set of type 7 was extracted from Tanner and is shown in Figure 87 along with the following 4 different MV curves: (1) same as shown on page D-75 (using entire set and measured value of  $B_0$ ), (2) same as 1 except that the lag (i.e., initial 3 data points) was excluded from the regression analysis, (3) same as 1 except that the optimum value of  $B_0$  was used (i.e.,  $B_0$  was selected so as to minimize  $\sum(t-t_{calc})^2$ ), and (4) same as 2 except that the optimum value of  $B_0$  was used. Examination of these 4 curves yields the following conclusions: (1) even though the lag is slight with a gradual transition into the exponential growth phase, allowing reasonable representation of the entire data set by the MV model, markedly better results are obtained when excluding the lag portion from the regression

Figure 87



Source : Tanner, R.D. (data set #1) ; refer to pages D-74 & D-75

Figure 88



Source : Wong, P.T., Lu, D. & Dutka, E.J. (refer to data set #1 on p.D-82/83)

analysis, and (2) while biomass determination via optical density measurements yields reasonable results in this case, the variable-biomass effect is again underpredicted as a result of the method measuring total (instead of active) biomass concentration. Tanner presented this data set as preliminary support for a proposed, mechanistically-more-complex model.

The last batch reactor data set to be discussed for single-culture systems is from Wong, Liu and Dutka (refer to Figure 88). The transition from lag to biodegradation is too sharp to be well represented by the MV model shown on page D-88. Best results are obtained by neglecting the lag during the kinetic analysis. The first-order model, for example, is shown to well fit the remaining points. No kinetic analysis was performed by the authors of this data set.

### 6.3 Continuous Stirred-Tank Reactor Data

Only 8 of the 148 biodegradation data sets studied in this thesis were obtained using continuous stirred-tank reactors (i.e., CSTRs). This is attributed to the fact that CSTRs are more difficult to set up, run and obtain reliable measurements. The use of CSTRs for the study of biodegradation poses certain advantages, however, over batch reactors: (1) the kinetic analysis is simpler involving only algebraic manipulations (vs. calculus for batch reactor data analysis), and more importantly (2) almost all industrial and municipal wastewater treatment facilities operate in the continuous mode (as opposed to batch). Laboratory studies in CSTRs, therefore, provide a better manner with which to measure and predict the biodegradation reactor's performance on large scale.

The kinetic expressions derived in Appendix B are for ideal CSTR behavior and require that the following assumptions be met by laboratory-scale units in order for the equations to be theoretically valid: (1) substrate concentration,  $S_e$ , vs. residence time,  $(V/Q)$ , measurements are made under steady-state conditions, (2) constant reactor volume is maintained, and (3) the composition of substrate and biomass is uniform throughout the reactor. The first and second assumptions can generally be met. However, even with effective mixing and aeration, wall growth can nullify the third assumption, unless the reactor walls are periodically scrubbed down. For biodegradation kinetics which are typically of fractional order, the assumption of perfect (micro) mixing for design purposes will result in the prediction of higher substrate conversions than that of the segregated-flow (macromixing) approach.<sup>7</sup> This, in turn, can result in the undersizing of a plant-scale, wastewater-treatment reactor. The segregated flow approach, however, is experimentally and analytically more difficult and the resulting improvement in results may, in many cases, only be marginal.

The characteristic  $S$  vs  $t$  curves shown in Figure 1 on page 20 for batch-reactor data sets are not applicable to CSTRs. The corresponding characteristic effluent substrate concentration,  $S_e$ , vs residence time,  $(V/Q)$ , curves for CSTRs are shown in Figures 89-94 for the zero-order, first-order and Monod expressions presented in Table 2 on page 15. The variable-biomass versions shown in Figures 90, 92 and 94 assume  $B_e$  to equal  $(B_i + Y_c(S_i - S_e))$ , which for sterile feeds (i.e.,  $B_i = 0$ ) reduces to  $(Y_c(S_i - S_e))$ . These relationships do not apply when either wall growth occurs or sludge is recycled (i.e., they are valid only for a chemostat). It should be noted that both the constant- and variable-biomass, lower-parameter models allow regression to include data points in which  $S_i$  is varied in addition to  $(V/Q)$ . The  $S_e$  vs  $(V/Q)$  curves, however, can only be graphically presented for the case in which  $S_i$  is held constant.

Figure 89 shows the zero-order, constant-biomass relationship for a CSTR to be analogous to that for a batch reactor. The model in both cases predicts substrate concentration ( $S_e$  or  $S$ ) to drop linearly with time (i.e., residence time for a CSTR), and for conversion to be complete after a fixed time period (i.e.,  $S_i/K$  or  $S_o/K$ ). The  $S_e$  vs  $(V/Q)$  curve for zero-order, variable-biomass kinetics in a CSTR, however, is different from that for the batch reactor (e.g., compare Figure 90 with Figure 39). Figure 90 shows the rate of conversion to decrease with residence time before ultimately becoming complete at a time equal to  $S_i/(k_o(B_i + Y_c S_i))$ .



Figure 89

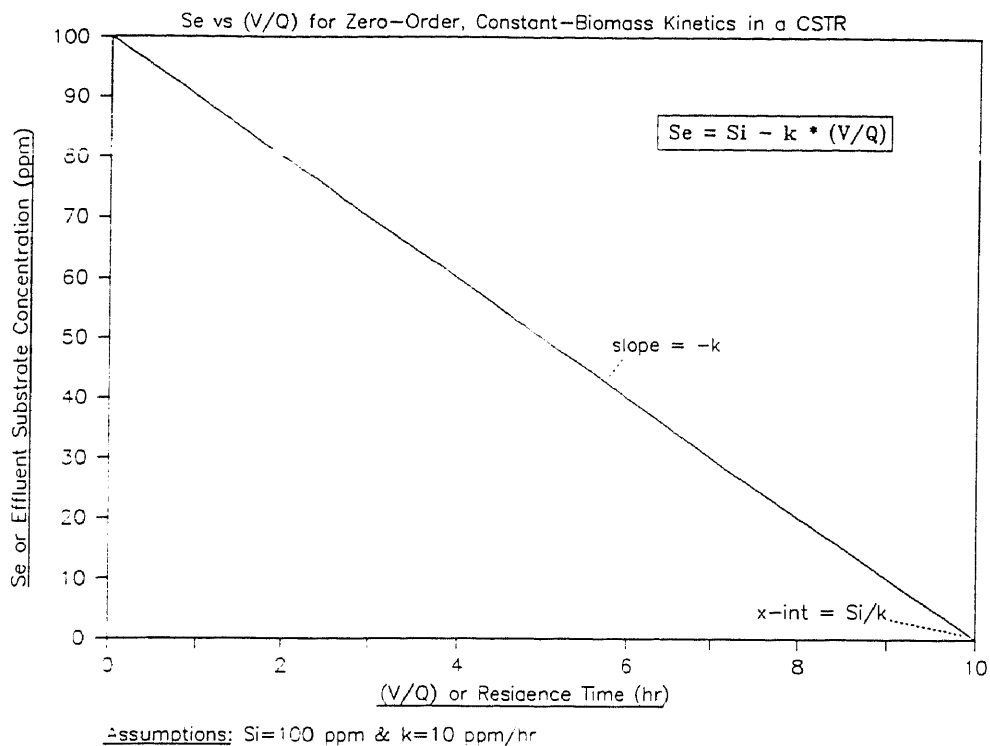


Figure 90

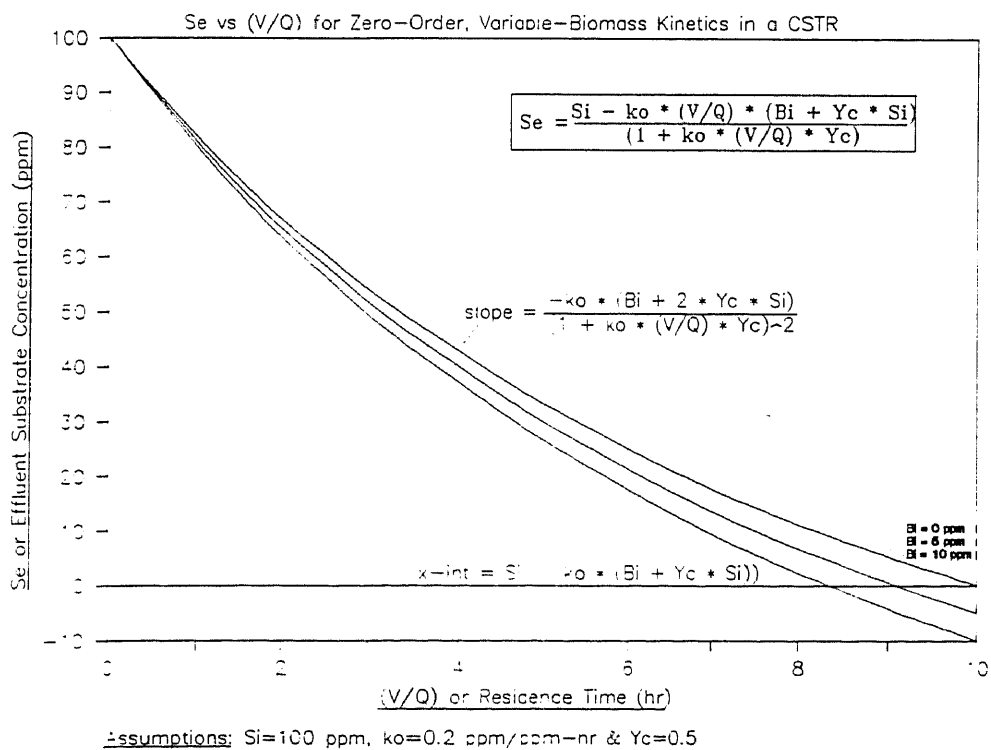


Figure 91

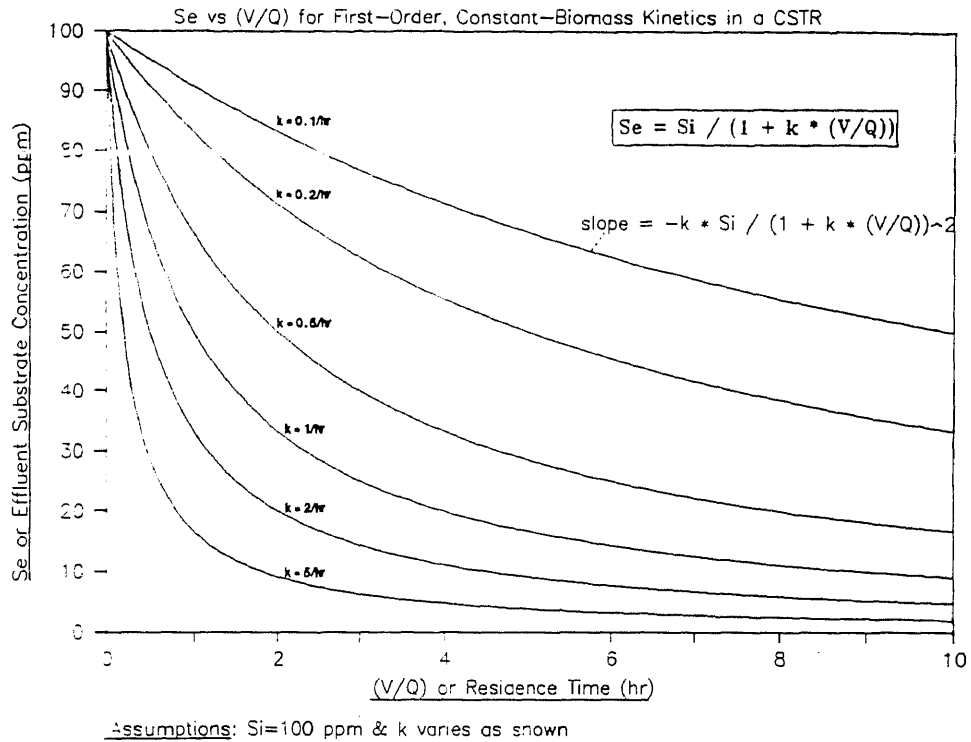


Figure 92

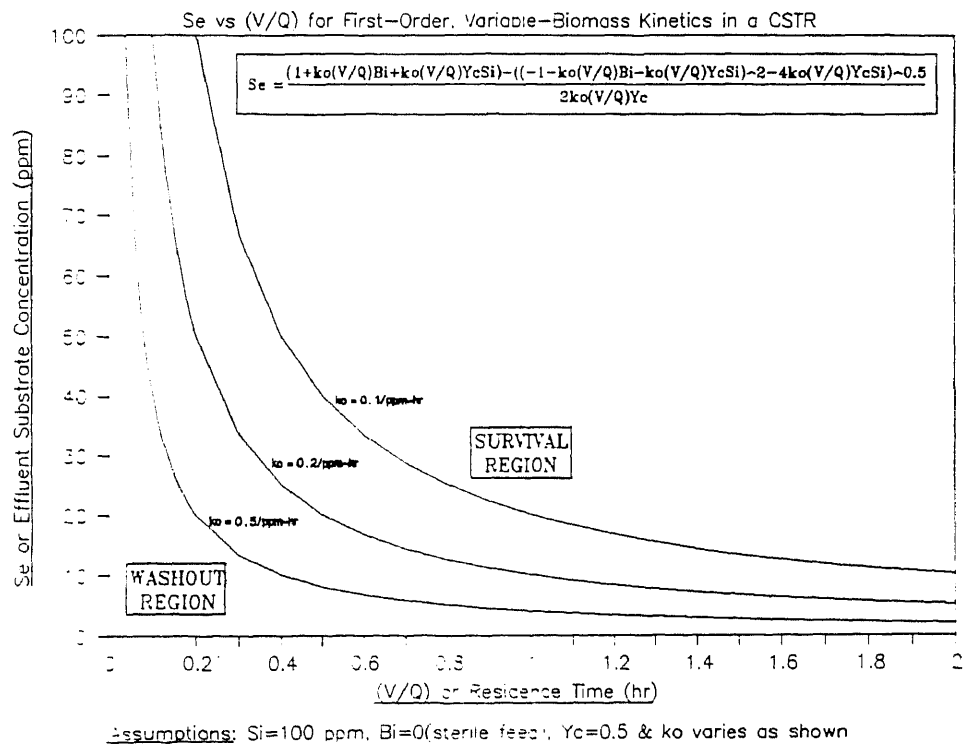


Figure 93

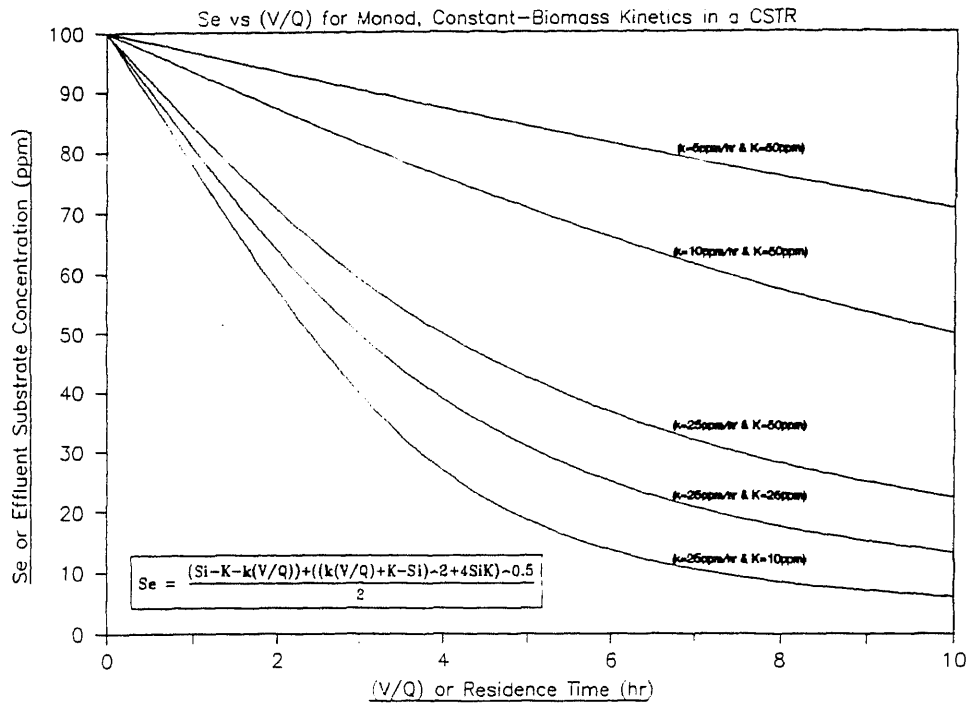
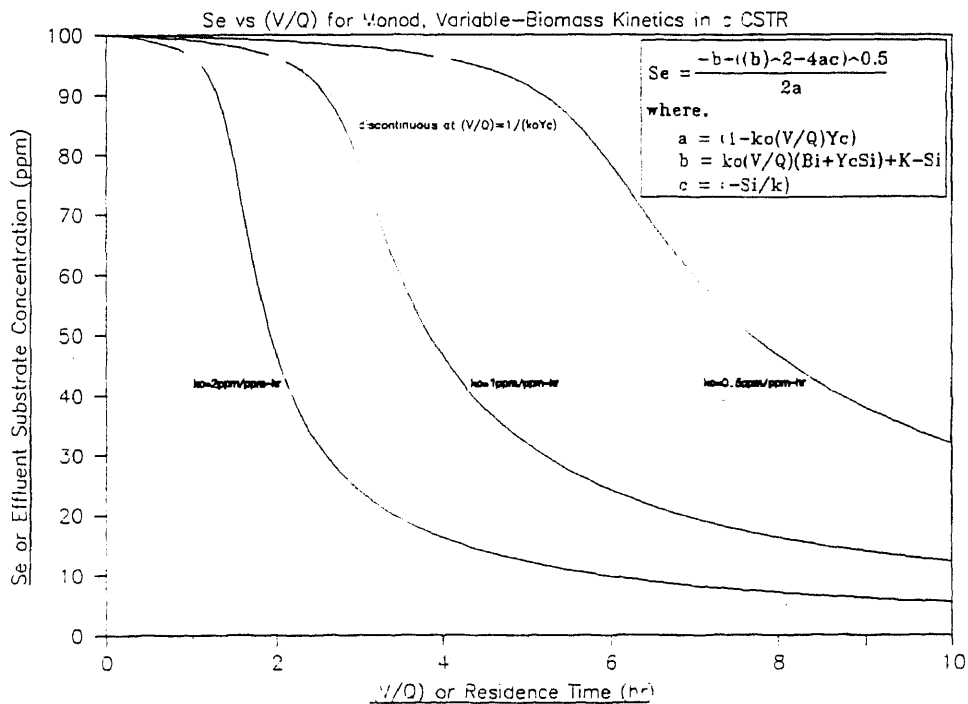


Figure 94



Figures 91 and 92 graphically present the characteristic  $S_e$  vs  $(V/Q)$  curves for the case of first-order kinetics in a CSTR. Of particular interest in Figure 92 is that (for the kinetic parameters arbitrarily selected) no conversion of substrate is obtained below certain residence times when operating under steady-state conditions. This is due to the physical phenomenon known as washout and occurs when the rate of loss of biomass in the effluent exceeds its generation rate. Figure 92 shows that washout occurs at progressively lower residence times as the rate of substrate utilization increases.

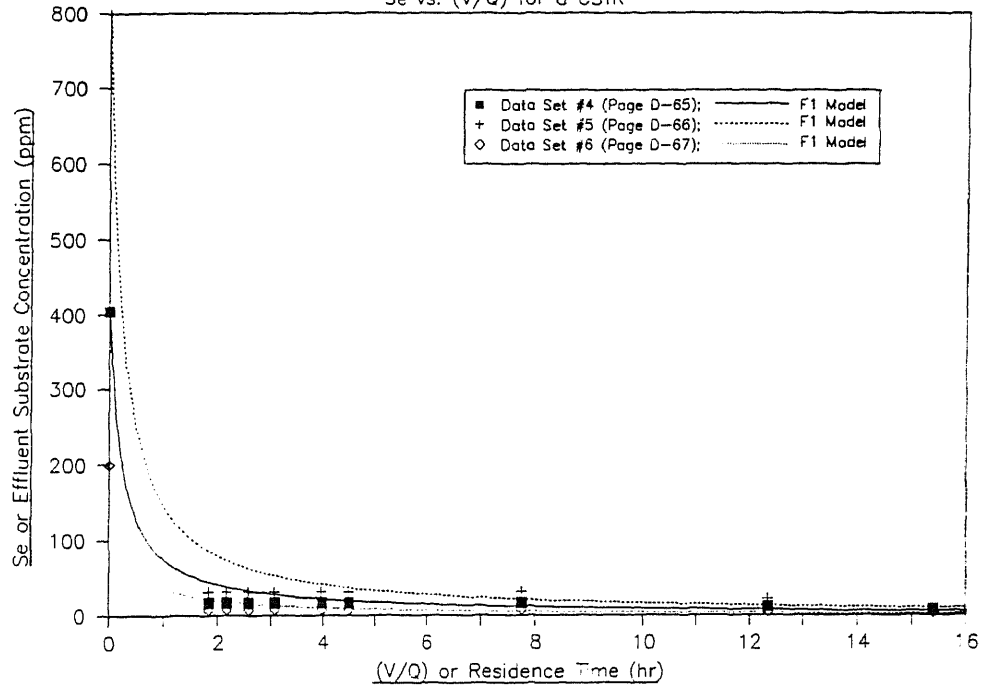
The characteristic  $S_e$  vs  $(V/Q)$  curves for Monod kinetics in CSTRs are graphically shown in Figures 93 and 94. The curves are visually analogous to those for ideal batch reactors. It should be noted that the  $MV$  curves in Figure 94, however, are discontinuous for a CSTR at values of  $(V/Q)$  equal to  $1/(k_o Y_c)$ . This is not an actual physical phenomenon but rather a mathematical artifact of the quadratic equation used.

The 8 CSTR data sets studied in this thesis were extracted from 4 different articles. The discussion of the results from each article is handled separately within this section because of inherent differences in CSTR operation by the different authors.

Figure 95 presents 3 CSTR data sets which were extracted from Radhakrishnan and Sinha Ray. Whereas the authors presented biomass concentration data for these sets, the variable-biomass models were not

Figure 95

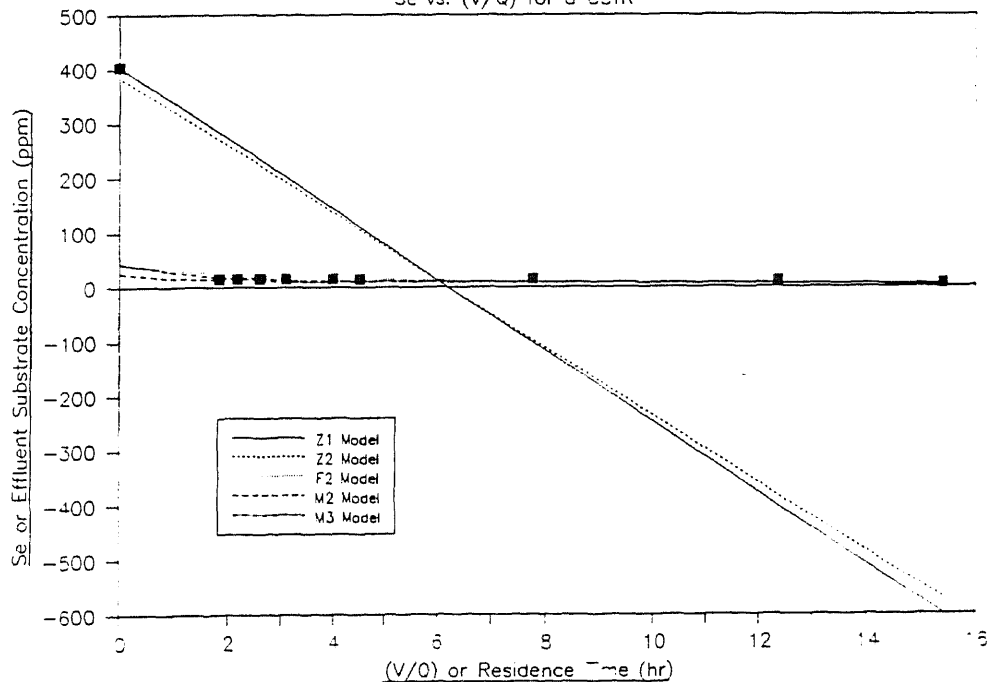
Se vs. (V/Q) for a CSTR



Source : Radhakrishnan, I. & Sinha Ray, A.K. (phenol substrate in B.cereus)

Figure 96

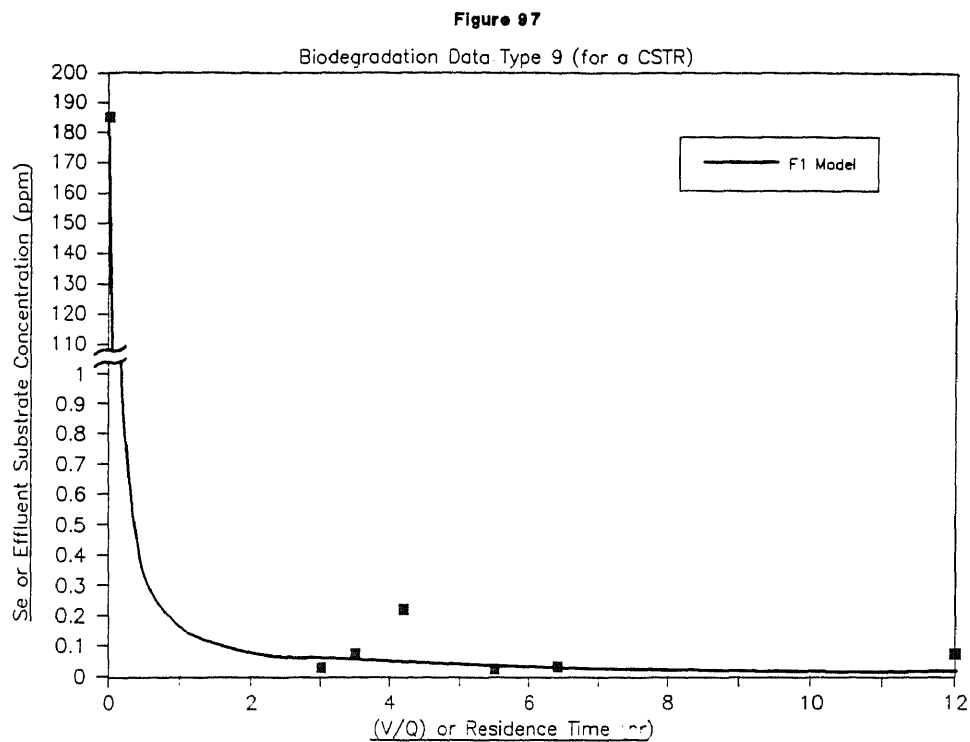
Se vs. (V/Q) for a CSTR



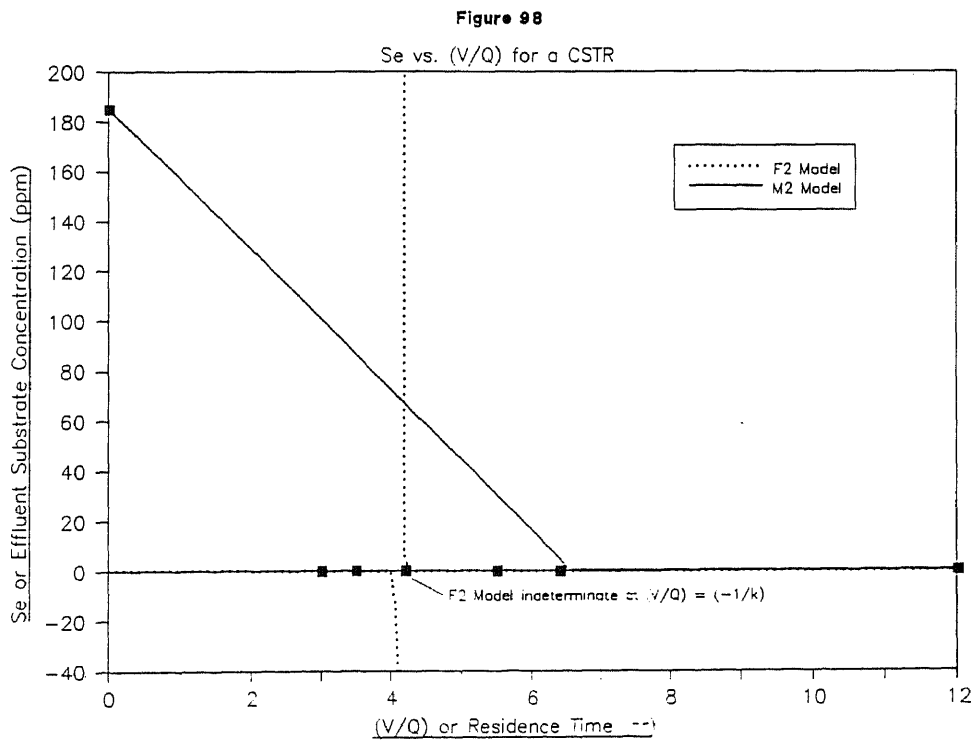
Source : Radhakrishnan, I. & Sinha Ray, A.K. (data set #4 from page D-65)

evaluated in Appendix D because the measured biomass concentration was constant for each set over the range of residence times covered. The F1 curves are visually the best of the models evaluated and are shown for each of the 3 sets in Figure 95. For comparison sake, Figure 96 shows the other 5 regressed curves for only one of the 3 sets since the general performance characteristics for all 3 are comparable. The M2 and M3 models regress negative values of both  $k$  and  $K$  in each case because of the data apparently dropping at greater-than-first-order rate (i.e., biodegradation data type 8), which is analogous to batch reactor behavior. None of the models evaluated in this thesis are capable of adequately representing these sets. The authors noted that  $Se$  and  $Be$  remained constant over the residence times covered possibly because of sensitivity limitations on the analytical methods. They also noted that neither the Michaelis-Menten relation nor the Tissier equation (i.e.,  $\mu = \mu_m(1 - \exp(\text{constant} * Se))$ ) hold for the measured data. Measurements for lower residence times would have provided greater insight into the kinetic behavior of these data systems. It should be noted that the authors made no mention as to the validation of the perfect mixing assumption of their CSTR via residence time distribution studies and, as such, the validity of the data for kinetic analysis purposes must be questioned.

Figure 97 presents a data set from Hill and Robinson which is analogous to those in Figure 95 in that  $Se$  is very low and virtually constant (within the apparent accuracy of the analytical method) over the residence time tested. Again, F1 is the visually best model and is



Source : Hill, G.A. & Robinson, W.R. (data set #2 on pages D-32 & D-33)



Source : Hill, G.A. & Robinson, W.R. (data set #2 on pages D-32 & D-33)

presented in Figure 97. Unlike the data sets in Figure 95, however, this data set causes all of the Monod models to regress negative values of  $K$  only (i.e.,  $k$  is positive in each case). This is attributed to the data point at a residence time of 4.2 hr which has a value of  $S_e$  that is an order of magnitude higher than the others (refer to pages D-32 and D-33). Not only does this abnormally high value of  $S_e$  cause the Monod models to regress negative values of  $K$ , but it also causes the F2 model to regress a negative value for  $k$ . Figure 98 graphically presents the M2 and F2 curves for this data set.

Hill and Robinson performed residence time distribution studies to confirm that their laboratory CSTR exhibited perfectly mixed behavior in the liquid phase over the range of feed and aeration rates used. The authors, however, did not confirm whether measurements were truly made under steady-state conditions. They stated that their measurements may only have been transient phenomena as their runs often had to be cut short because of observed wall growth. The lack of model-predicted response in  $S_e$  by the authors (i.e., they evaluated substrate-inhibition models) was attributed by them to be due to either small variations in the feed rate or undetected, localized wall growth. Wall growth has long been known to affect measurement of kinetic parameters and process stability.

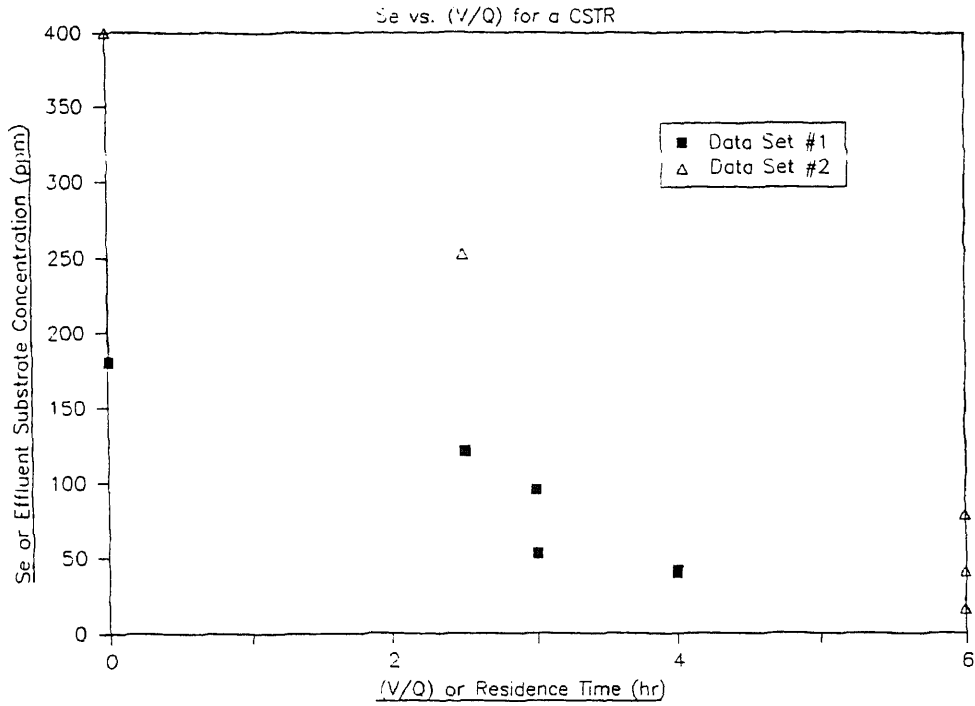


It should be noted that Hill and Robinson used sterile feed (i.e.,  $B_i=0$ ) and measured  $B_e$ , which is theoretically equal to  $Y_c(S_i-Se)$ , directly. The measured values of  $B_e$  varied only slightly as the variable-biomass models closely approximated the lower-parameter, constant-biomass models. Because  $B_e$  did, however, vary (even if only slightly) from data point to data point, and not exactly as per the relationship  $Y_c(S_i-Se)$ , the  $Se$  vs  $(V/Q)$  plot does not result in smooth curves for the variable-biomass models with this data set (i.e.,  $Se$  becomes a function of  $B_e$  in addition to  $(V/Q)$ ).

The remaining 4 CSTR data sets to be discussed are from 2 articles with the same principle author (i.e., Beltrame, P.). CSTR operation was reported to be the same in both cases. Sterile feed (i.e.,  $B_i=0$ ) was used along with sludge recycle such that the measured value of  $B_e$  did not conform to the theoretical value of  $Y_c(S_i-Se)$ . Whereas the assumption of steady-state behavior was confirmed by the authors through repeated measurements, no mention was made of their checking the validity of the assumption of perfect mixing in their laboratory set-up.

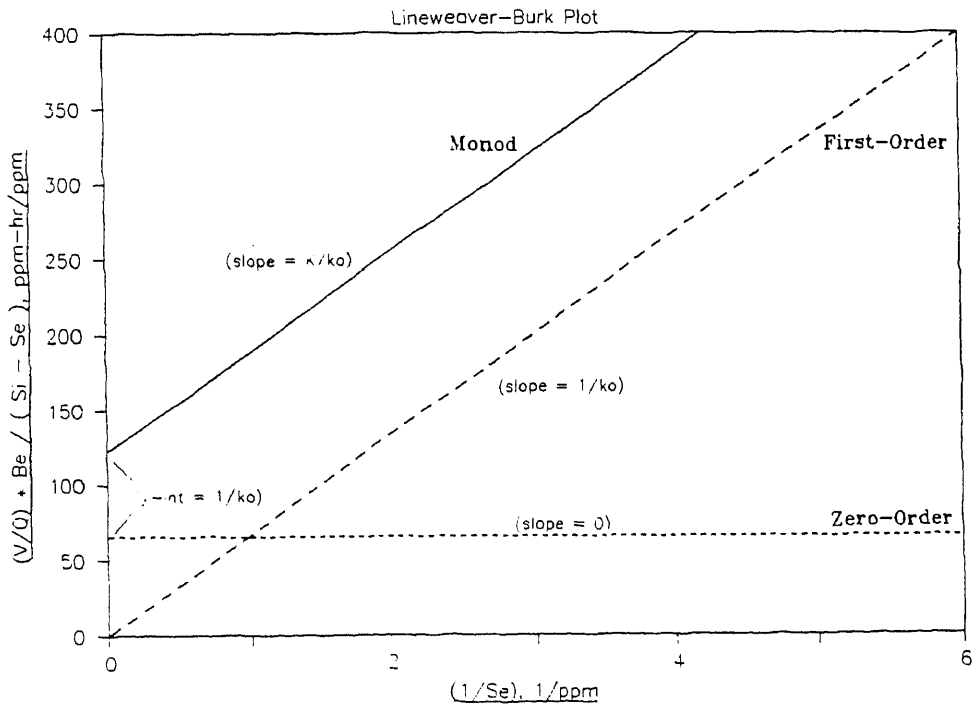
Figure 99 presents the  $Se$  vs  $(V/Q)$  plot for 2 CSTR data sets from Beltrame, P., et al (1984). The observed scatter in both data sets is due to significant variations in  $B_e$  measurements throughout the runs (refer to pages D-13 and D-15). Because  $B_e$  varies independently of  $S_i$  and  $(V/Q)$  for these data sets due to the authors' use of sludge recycle, plots of  $Se$  vs  $(V/Q)$  are of no practical value here. For these cases, the Lineweaver-Burk plot (i.e., a plot of  $((V/Q)B_e)/(S_i-Se)$  vs  $(1/Se)$ )

Figure 99



Source : Beltrame, P., et al (1984); data sets #1 & #2 on pages D-12..D-15

Figure 100



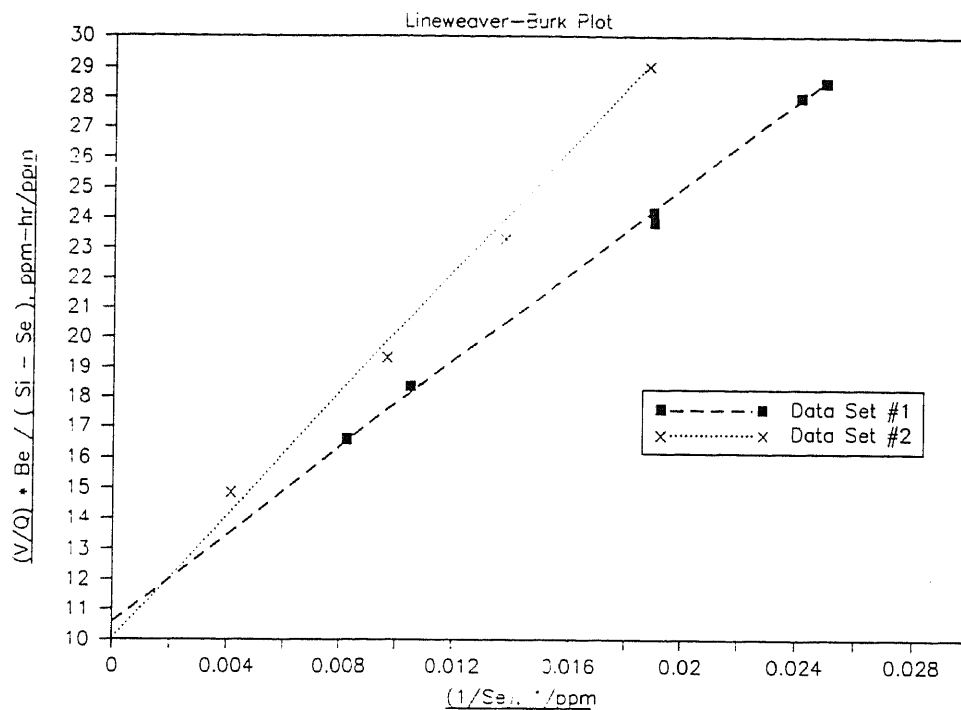
is preferred. Figure 100 shows the expected characteristic linear relationships of a Lineweaver-Burk plot for zero-order, first-order and Monod kinetics. Data sets #1 and #2 from Figure 99 are shown to be well represented by the Monod model on the Lineweaver-Burk plot in Figure 101. The regression results for these 2 data sets on pages D-12 through D-15 show the MV model to be best. M2 and M3 regresses negative values of both  $k$  and  $K$  while F2 regresses negative values of  $k$  for both data sets.  $B_e$  is seen to vary too much from data point to data point (due to sludge recycle) for the data sets to be well-represented by the constant-biomass models.

The regressed results from pages D-13 and D-15 for the MV models are in good agreement with those performed by the authors. A comparison is provided below:

|             | <u>Results from Appendix D</u>                 |                             | <u>Results from Article</u>                    |                             |
|-------------|--|-----------------------------|--|-----------------------------|
|             | <u><math>k_o</math> (<math>hr^{-1}</math>)</u> | <u><math>K</math> (ppm)</u> | <u><math>k_o</math> (<math>hr^{-1}</math>)</u> | <u><math>K</math> (ppm)</u> |
| Data Set #1 | 0.0935   | 66.35                       | $0.094 \pm 0.003$                              | $67 \pm 2$                  |
| Data Set #2 | 0.0997   | 98.20                       | $0.095 \pm 0.007$                              | $91 \pm 9$                  |

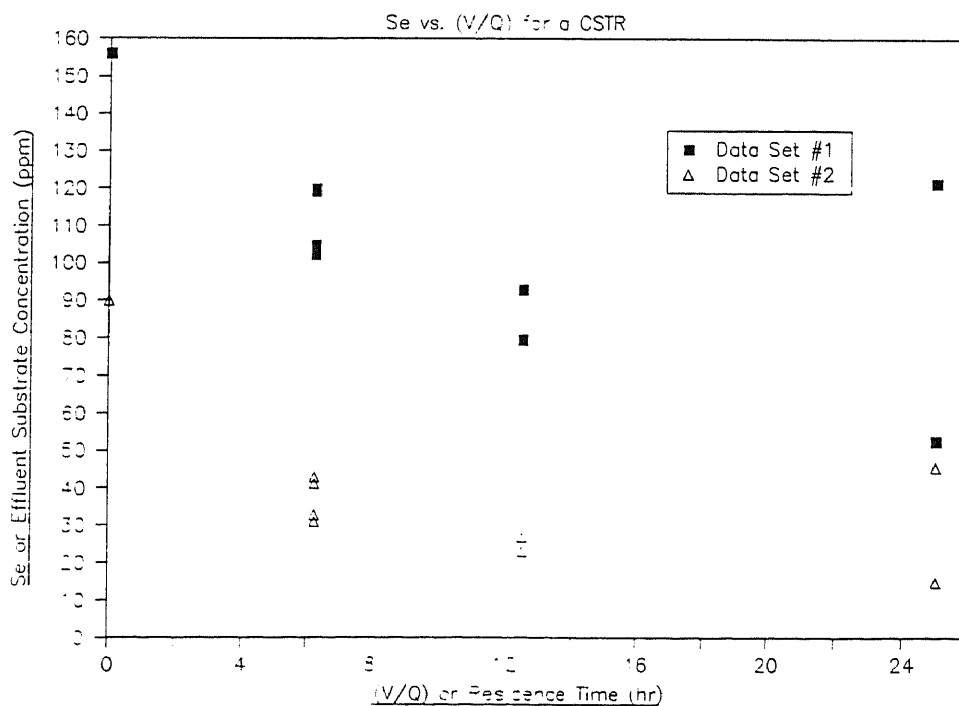
While  $k_o$  is the same within experimental error for the 2 sets,  $K$  differs due to substrate-inhibitory related effects which are accounted for by the authors of this article in a model by redefining  $K$  as a linear function of  $S_e$  (i.e.,  $K = K_1 + K_2 * S_e$ ).

Figure 101



Source : Beltrame, P., et al (1984); data sets #1 & #2 on pages D-12..D-15

Figure 102



Source : Beltrame, P., et al (1982); data sets #1 & #2 on pages D-16..D-19

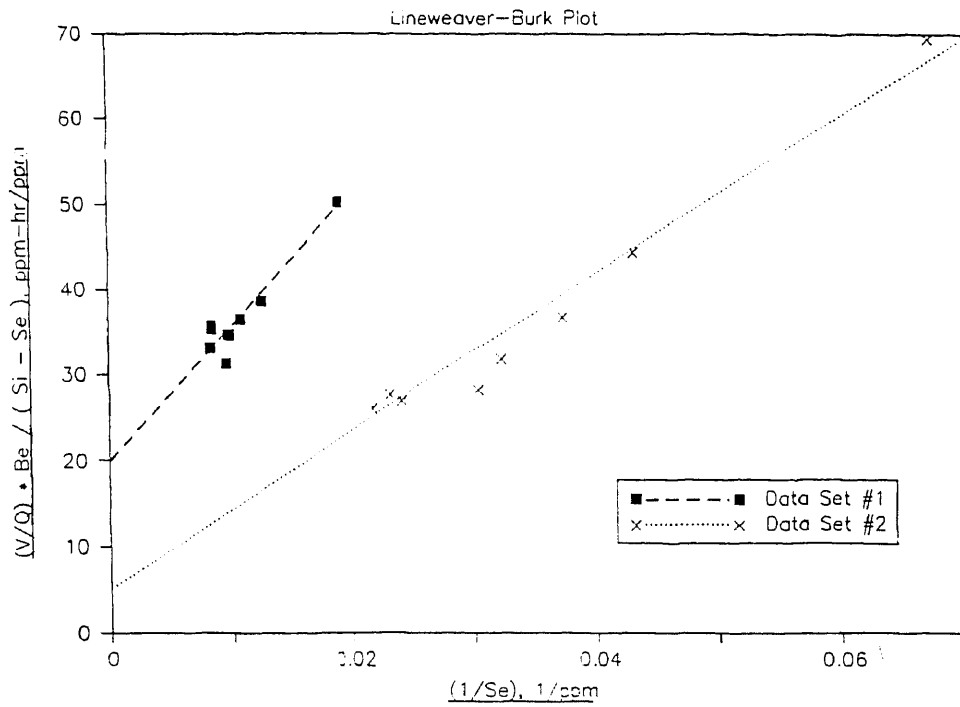
Figure 102 shows a  $S_e$  vs.  $(V/Q)$  plot for 2 data sets from the other Beltrame article (i.e., from 1982) which is similar to those sets shown in Figure 99 with respect to data scatter being present due to significant variations in  $B_e$  (refer to pages D-17 and D-19). Figure 103 graphically shows the corresponding Lineweaver-Burk plots for the 2 data sets to be reasonably linear. While the MV model is best for both cases, the FV model is not much worse for data set #2 (refer to page D-19). The authors used the FV model to represent data set #2 and the MV model for data set #1. The regressed results from pages D-17 and D-19 are shown below to be in fair agreement with the regressed results presented in the article.

|             | <u>Results from Appendix D</u>                 |                             | <u>Results from Article</u>                    |                             |
|-------------|--|-----------------------------|--|-----------------------------|
|             | <u><math>k_o</math> (<math>hr^{-1}</math>)</u> | <u><math>K</math> (ppm)</u> | <u><math>k_o</math> (<math>hr^{-1}</math>)</u> | <u><math>K</math> (ppm)</u> |
| Data Set #1 | 0.0498   | 77.87                       | $0.045 \pm 0.005$                              | $63 \pm 12$                 |
| Data Set #2 | 0.000933                                       | -----                       | $0.00098 \pm 0.00002$                          | -----                       |

#### 7. Analysis of the Effect of Experimental Error in Biodegradation Data on Kinetic Model Selection

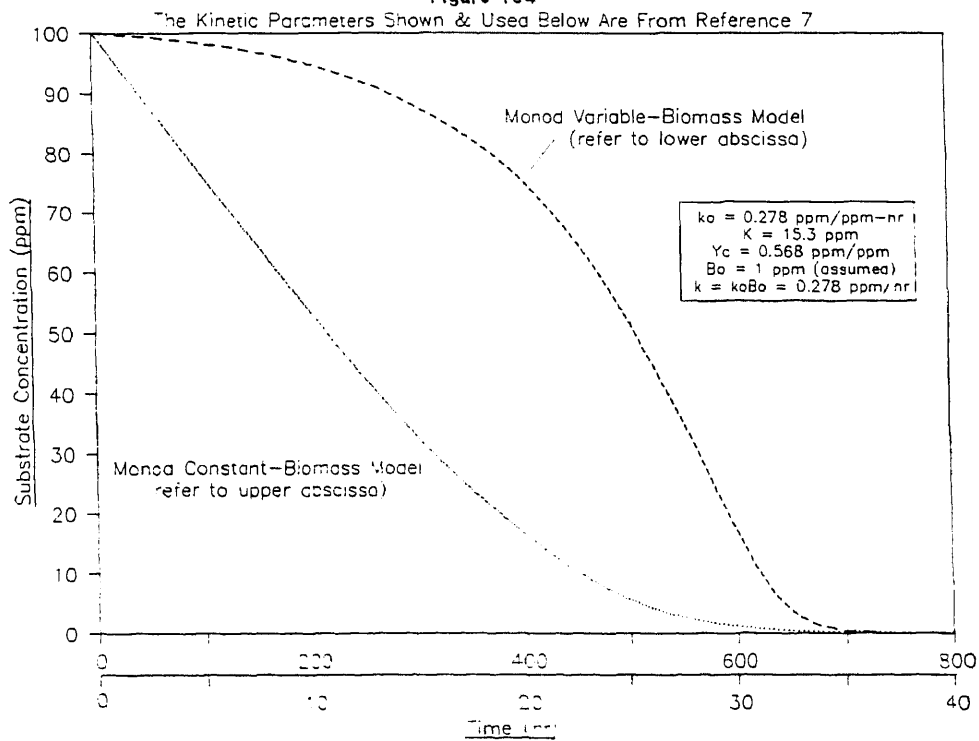
Section 6 comprehensively covered the kinetic analysis of raw aerobic biodegradation data from both batch reactors and CSTRs with respect to the constant- and variable-biomass versions of the zero-

Figure 103



Source: Beltrame, P., et al (1982); data sets #1 & #2 on pages D-16..D-19

Figure 104



order, first-order and Monod models. While the general characteristics (i.e., pros and cons) of each model for each given data type were discussed, only qualitative statements could be made as to the significance of data set quality on proper model selection. In this section, the effects of key biodegradation data measurement parameters on kinetic modelling will be systematically studied in an attempt to quantitate their impact. The ultimate goal of this effort is to establish concrete guidelines for the measurement of reliable biodegradation data for wastewater treatment reactor design purposes.

This study will be limited to the case of batch reactor data since: (1) batch reactors are commonly used for biodegradation data measurement (e.g., 140 of the 148 data sets evaluated in this thesis are from batch reactors); and (2) CSTRs have not been shown in this thesis to readily yield reliable kinetic data (refer to Section 6.3 for a description of the physical problems encountered with wall growth, imperfect mixing and achieving steady-state conditions in CSTRs). The biodegradation data measurement parameters evaluated herein in terms of their effect on proper kinetic model selection are: (1) random experimental error in  $S$  measurements, (2) number of  $S$  vs  $t$  data points, (3) data spacing/grouping, and (4) data range/truncation. While accurate measurement of biomass concentration has been repeatedly stressed within this thesis as necessary for the regression and application of the variable-biomass models, it is not assessed here because the errors in its measurement are primarily systematic (rather

than random) in nature. A discussion of the importance of accurate values of  $B_0$  and  $Y_c$  (as well as the sensitivity of regression analysis to these parameters) has been covered in sufficient detail in Section 6.

### 7.1 Methodology

As stated previously in Section 6.1, most batch reactor data types are some variation of one of the two  $S$  vs  $t$  curves shown in Figure 1. Both of the curves can be well represented by the Monod models (i.e., M2 or M3 for Curve 1 and MV for Curve 2). As a result, the Monod models are used here as the basis for the systematic study of the effect of the experimental error and other data measurement parameters on proper kinetic model selection. It is assumed here that the "real"  $S$  vs  $t$  biodegradation data (from which abiotic mechanisms are assumed to have been excluded) are exactly as represented by the two Monod models shown in Figure 104 for the two cases of constant- and variable-biomass behavior. The kinetic parameters used as a basis for the curves presented in Figure 104 are for phenol using Pseudomonas putida and are as follows (note:  $B_0$  is assumed to be 1 ppm in both cases):<sup>8</sup>

$$\begin{aligned}k_o &= (\mu_m/Y_c) = (0.158/\text{hr})/(0.568 \text{ ppm/ppm}) \\&= 0.278 \text{ ppm/ppm-hr}\end{aligned}$$

$$K = 15.3 \text{ ppm}$$

$$k = k_o B_0 = (0.278 \text{ ppm/ppm-hr})(1 \text{ ppm}) = 0.278 \text{ ppm/hr.}$$



This system was selected as the basis for this study because phenol is a commonly-encountered, well-studied substrate and Pseudomonas putida is a commonly-found culture in activated sludge with known activity toward phenol utilization. The phenol concentration range was assumed to be 0.1-100 ppm, since that would cover most applications of practical interest.

This study basically involves the following: (1) assuming the two curves in Figure 104 represent the "real" S vs t data that would be measured under ideal circumstances, (2) extracting discrete points from the two curves and adding random experimental errors to each, (3) varying the biodegradation data measurement parameters listed in Section 7, and (4) assessing their impact on the regression analysis results. The effect of each parameter on proper kinetic model selection can be assessed either graphically (i.e., by comparing the predicted vs the ideal S vs. t curves) or analytically (i.e., by either comparing the regressed rate constants vs. those of the ideal case or by using the statistic  $\Sigma(t_{\text{predicted}} - t_{\text{real}})^2$ ). For the ideal case, the predicted S vs t curve will be identical to the "real" one, with  $k_0$  and K being the same in both cases and  $\Sigma(t_{\text{predicted}} - t_{\text{real}})^2$  being zero.

A brief discussion as to the manner in which the random experimental error was added to the discrete points from the "real" curves (from Figure 104) follows here prior to proceeding with a discussion of the results. First, a hundred equally spaced points (with respect to time) were extracted from each of the two curves in Figure 104 for the range of S from 100 ppm down to 0.1 ppm (refer to pages F-3 and F-4 in Appendix F for a tabulation of both of these sets). The IBM PC Basic program "Randomize" was then used to generate a hundred points at random between the range of 0 and 1 (refer to page F-5 for this tabulation). Figure 105 graphically displays the distribution of these randomly-generated numbers in bar-chart form. The sample of randomly-generated points taken is large enough (i.e., 100 points) such that the distribution is observed to be fairly equally spread over the range covered.

The randomly-generated points on page F-5 were then assumed to equal P(u) of the cumulative normal probability distribution:

$$P(u) = \int_{-\infty}^u (2\pi)^{-0.5} \exp(-(u')^2/2) du'; \quad (5)$$

where,

P(u) = probability (expressed in fraction form) of a  
sample from a normal distribution with standard  
deviation u' having a value of less than u.

u' = standard deviation

u = deviation from mean in standard deviation units

Figure 105

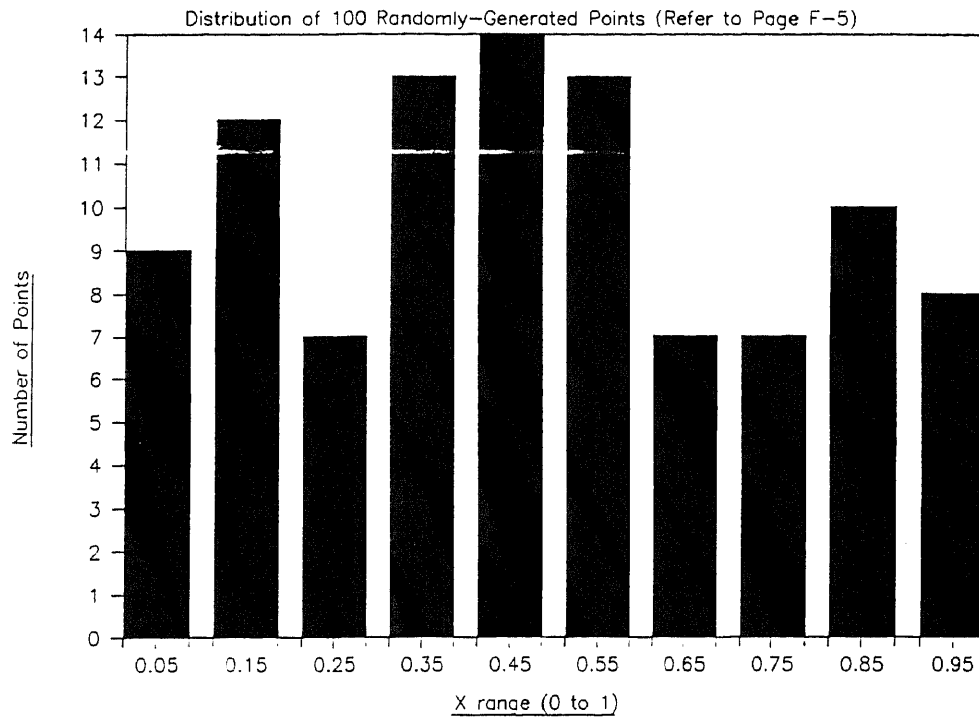
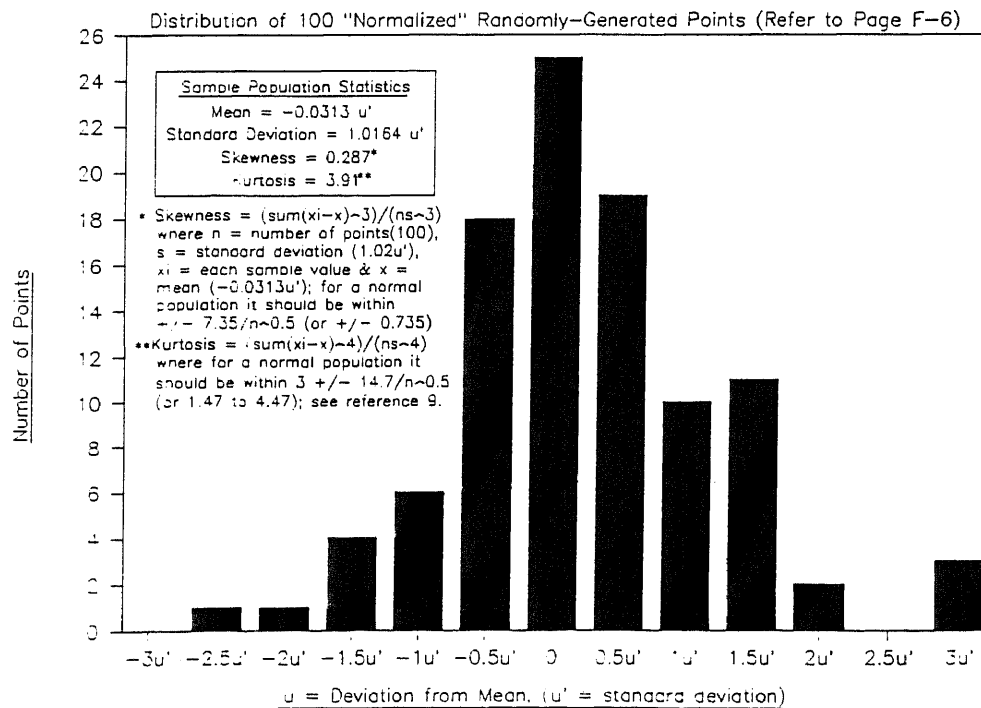


Figure 106



For each of the 100 points on page F-5, the value of  $u$  from the above expression was determined using a cumulative standard normal probability distribution table. The corresponding tabulation of  $u$  values are presented on page F-6. Figure 106 graphically presents this "normalized" random distribution in bar-chart form. The distribution of points well approximates the normal distribution function with the calculated values of the mean and standard deviation for the sample set being close to ideal (i.e., 0 and 1  $u'$ , respectively). Furthermore, two quantitative tests prescribed by Holmes<sup>9</sup> (i.e., for skewness and kurtosis) to check the normality of a population were applied to the set of points from page F-5. The results (shown on Figure 106) meet the criteria established by Holmes for a normal distribution.

The above, normalized distribution was assumed in this study to represent the random error in  $S$  experienced during experimental measurement. Different levels of accuracy were assessed in this analysis by assuming different values of  $u'$ . In each case, the hypothetically measured value of  $S$  was determined by adding the value of  $u$  from page F-6 (which is first multiplied by the assumed value of  $u'$ ) to the corresponding "real" value of  $S$  from either pages F-3 or F-4. In this manner, the effect of random error in  $S$  was able to be studied (with respect to kinetic model performance) in a controlled fashion.

## 7.2 Discussion of Results

The effect of the total number of data points on regression results was evaluated for the case in which no experimental error was introduced to the two data sets on pages F-3 and F-4. For both data sets, regression analyses were performed (for the S range from 100 ppm down to 0.1 ppm) for each of the following number of equally-spaced (i.e., with respect to time) data points: (A) 100, (B) 34, (C) 12, (D) 10, and (E) 4. The results are presented on pages F-7 through F-12.

For the case in which constant-biomass behavior was assumed (i.e., the data set from page F-3), the effect of the total number of data points (down to a minimum of 4 data points) on the regression results can be seen on pages F-7 through F-9 to be insignificant for the case of "perfect" data (i.e., no experimental error present). The slight improvement in performance (in terms of  $\Sigma(t-t_{calc})^2$  and the regressed values of  $k_0$  and  $K$ ) as the number of points is reduced is due to the fact that the latter points of the set are given only to two significant figures. This introduces error into the regressed values of  $k_0$  and  $K$ , which increases with the total number of points used from this latter portion of the data set.

Likewise, for the case in which variable-biomass behavior was assumed (i.e., the data set from page F-4), no significant effect of the number of data points on regression results is observed for the case of "perfect" data (i.e.,  $u' = 0$ ). The slight improvement in the performance of MV with decreasing number of data points is again attributed to the use of fewer points from the latter, less accurate, portion of the data set. It should be noted that, although no significant effect of the total number of data points on regression results is observed for "perfect" data, it is logical from a statistical perspective that improved regression results would be obtained for data containing random experimental error when the sampling population (i.e., number of data points) is increased (i.e., the more data points, the better the results). This is demonstrated later in this section.

The effect of random experimental error in S measurements was evaluated for the case of constant-biomass behavior on pages F-13 through F-15. Ten equally spaced (with respect to time) S vs. t data points spanning the S range from 100 ppm down to 0.1 ppm (from page F-3) were modified to include random experimental error using the corresponding correction terms from page F-6. The following six levels

of error were evaluated: (1)  $u' = 0.1$  ppm, (2)  $u' = 0.25$  ppm, (3)  $u' = 0.5$  ppm, (4)  $u' = 1.0$  ppm, (5)  $u' = 2.0$  ppm, and (6)  $u' = 5.0$  ppm. Figure 107 graphically presents the individual data points for each level of error along with the corresponding regressed M2 curves. It should be noted that the ninth data point of the set (i.e., for  $t = 657$  hr), upon being modified to include random experimental error, resulted in negative values of  $S$  for the cases in which  $u'$  was greater than or equal to 1.0 ppm. Since negative values of  $S$  are physically impossible, and because setting  $S$  equal to zero results in indeterminate calculations for the Monod models, these negative  $S$  values were arbitrarily set to a very small value of  $S$  (i.e., 0.01 ppm).

Figure 107 shows the regressed M2 models to become progressively worse as the level of random experimental error (i.e.,  $u'$ ) increases. For the  $S$  range of interest (i.e.,  $100 \rightarrow 0.1$  ppm), the regression results become notably worse for  $u'$  values greater than 0.25 ppm (refer to pages F-13 through F-15 for a comparison of  $\Sigma(t-t_{calc})^2$ ). It should be noted that Figure 107 only shows one of an infinite number of possible variations of random error distribution within the given data set. For consistently accurate regression results,  $u'$  should be less than the lowest absolute value

Figure 107

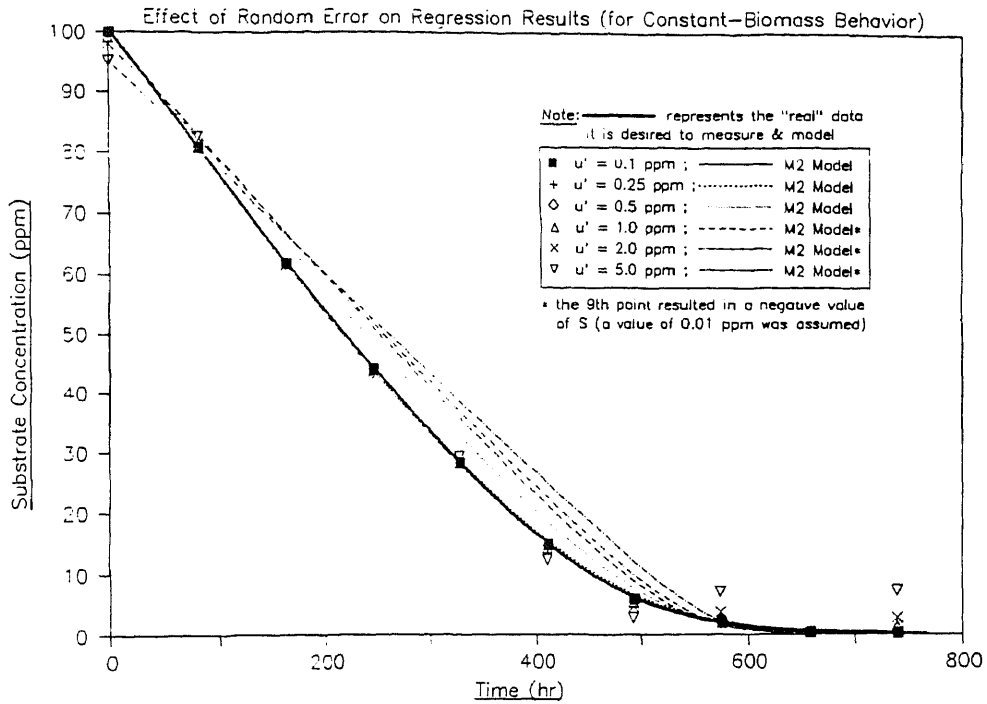
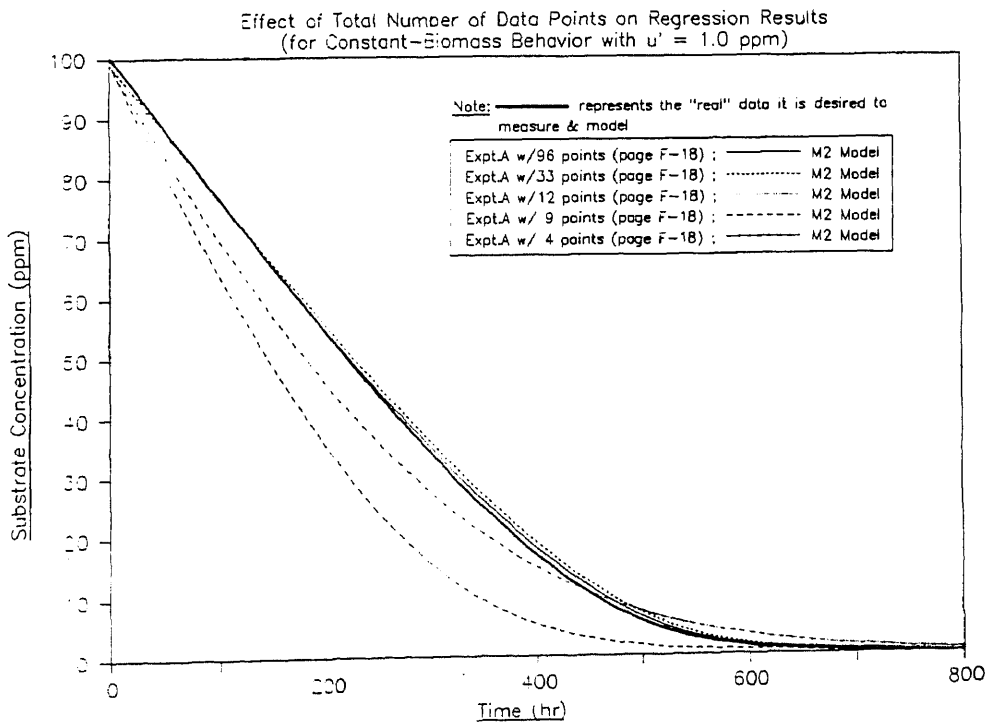


Figure 108





of  $S$  that is of interest. While increasing the number of data points will statistically result in an improvement in the accuracy of regression results for data with random experimental error (i.e.,  $u'$  not equal to 0), significant errors can be expected to be introduced in the regression results for values of  $S$  lower than  $u'$ . The effect of the total number of data points on the regression results for this data set with the following two levels of experimental error is shown on page F-18: (1)  $u' = 1.0$  ppm (refer to Figure 108), and (2)  $u' = 5.0$  ppm (refer to Figure 109). The performance of the models, as gauged by the % error in the rate constants, improves as expected with an increase in the frequency of sampling. The statistic,  $\Sigma(t-t_{calc})^2$ , is not as good a measure of overall performance as it only indicates the error in the measured points and not the entire curve. It should also be noted that the data points for which negative  $S$  values resulted (upon addition of the corresponding random error terms) were excluded from the analyses. This introduces systematic error into the analysis by, in effect, inflating the average  $S$  values which would otherwise be obtained in the latter portion of the curve. This is another reason why  $u'$  should be lower than the lowest value of  $S$  of interest for design purposes.

Figure 109

Effect of Total Number of Data Points on Regression Results  
(for Constant-Biomass Behavior with  $u' = 5.0$  ppm)

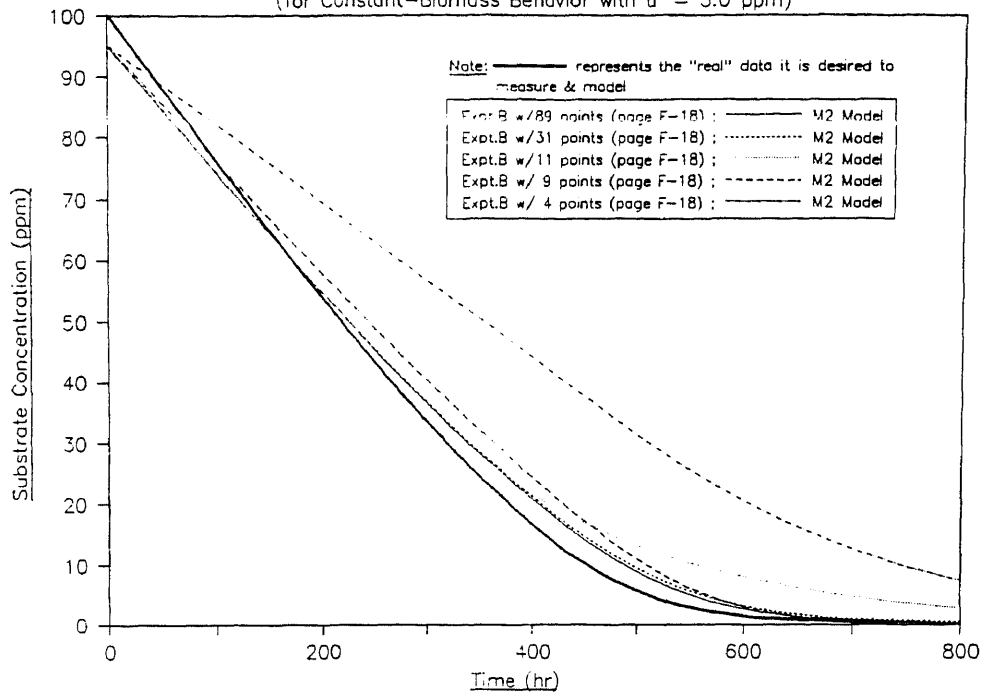
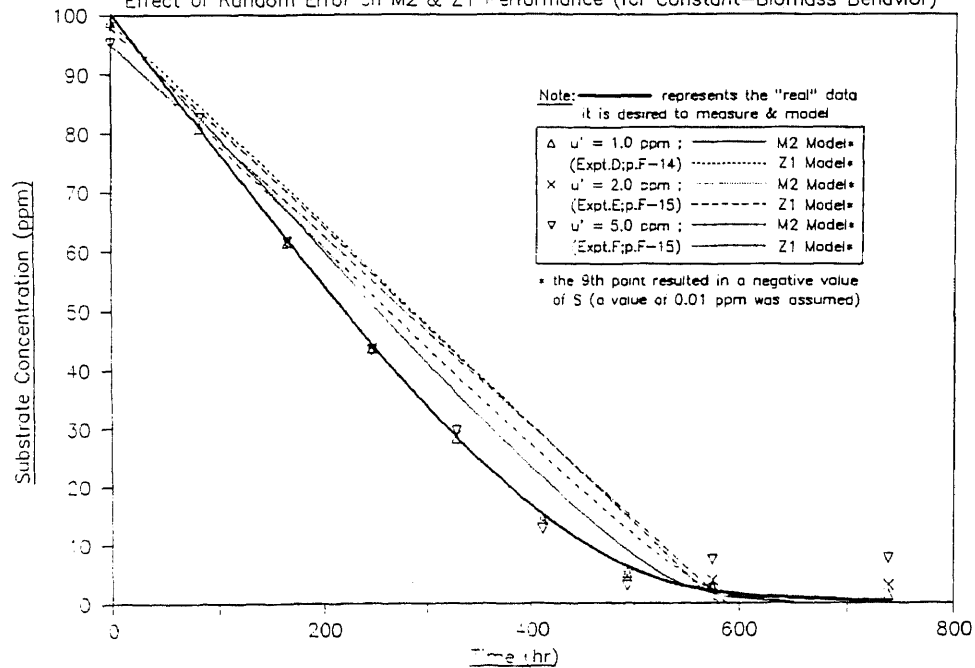


Figure 110

Effect of Random Error on M2 & Z1 Performance (for Constant-Biomass Behavior)



For the given distribution of random error in Figure 107, the constant-biomass Monod models become progressively worse as  $u'$  increases. The zero- and first-order constant-biomass models are worse (the latter much more so than the former) than the corresponding Monod models in each case, but less so on a relative basis as  $u'$  increases (refer to pages F-14 and F-15 for a tabulation of the results and to Figure 110 for a graphical presentation). The exact point at which the zero- or first-order model becomes comparable to the Monod model in performance cannot be generically predicted, but rather is a complex function of multiple parameters: (1) the system and its environment, (2) the  $S$  range covered, (3) the level of experimental error, and (4) the exact distribution of the random experimental error within the data set. For the case shown in Figure 110, the zero-order models statistically become comparable to the Monod models in performance for the case of  $u'$  equal to 5.0 ppm (note: the first-order models, however, are still much worse for this case and were, therefore, not included within Figure 110).

The effect of random experimental error in  $S$  measurements was evaluated for the case of variable-biomass behavior on pages F-16 and F-17. Ten equally spaced (with respect to time)  $S$  vs.  $t$  data points in the  $S$  range from 100 ppm down to 0.1 ppm (from page F-4) were modified to include random experimental error using the corresponding correction terms from page F-6. The same levels of experimental uncertainty were evaluated here as for the constant-biomass case.

Figure 111 graphically presents the individual data points for each level of error along with the corresponding MV curves. The performance of the MV models is seen to progressively worsen as  $u'$  increases. The MV model for error levels (i.e.,  $u'$ ) as low as 0.1 ppm is seen to deviate from the "real" curve for values of  $S$  below 25 ppm. This deviation increases for lower values of  $S$ . Figure 111 shows that  $u'$  should be well below the lowest value of  $S$  of interest for design purposes in order to obtain accurate results for systems with strong variable-biomass effects. For values of  $u'$  equal to 2.0 ppm, the performance of the MV model in terms of  $\Sigma(t-t_{calc})^2$  as shown on page F-17 has deteriorated to the point that the FV and ZV models perform comparably (refer to Figure 112 for a visual comparison of the MV, ZV and FV models for this case). The constant-biomass models are notably worse than MV for each of the  $u'$  values evaluated and they are not shown here. It should be noted that regression results for the case of  $u'$  equal to 5.0 ppm are indeterminate because of negative values within  $\ln$  functions. The function,  $f = B_0 + Y_c S_0 - Y_c S$ , is negative for the second point of the set, thereby making  $\ln (B_0 + Y_c S_0 - Y_c S)$  indeterminate for that point and, hence, the entire set for each of the three variable-biomass models.

As mentioned previously for the constant-biomass case, Figure 111 presents only one of an infinite number of possible variations for the distribution of random experimental error within the data sets. In general,  $u'$  should be less than the lowest value of  $S$  that is of interest for design purposes.

Figure 111

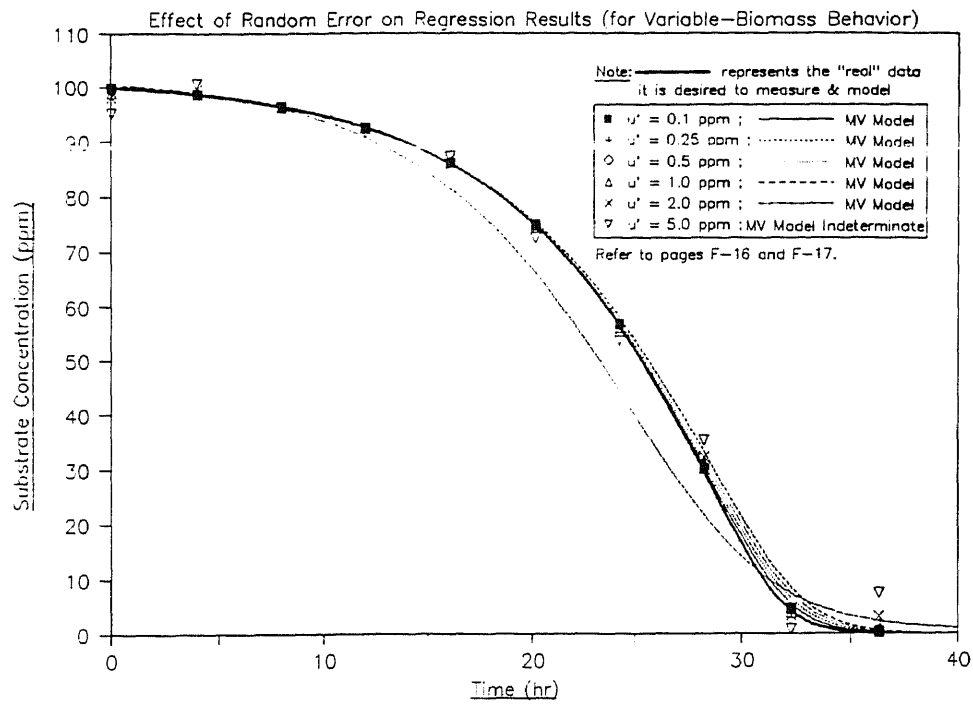
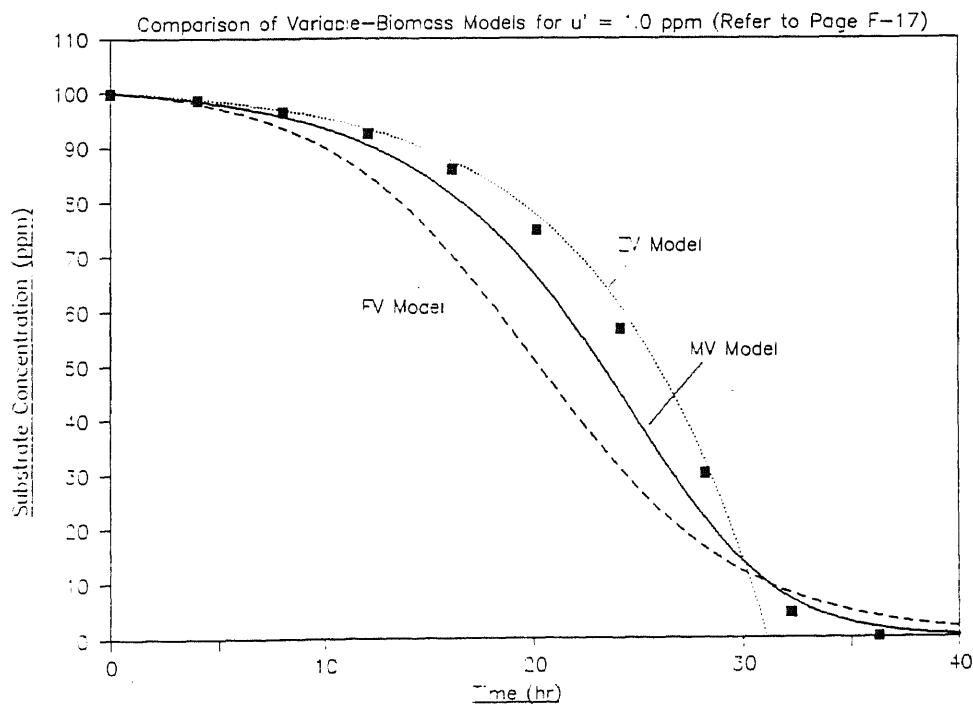


Figure 112



The effect of data spacing or regularity within a given S vs. t data set was evaluated on page F-19 for both constant- and variable-biomass kinetic behavior. Five different data spacings were assessed for each: (A) 9 points from the initial part of the set and the last point; (B) the first point and 9 points from the latter end of the set; (C) the first and last points with 8 points from the middle portion of the set; (D) 10 equally-spaced points with respect to time throughout the entire set; and (E) 10 randomly selected points from the set. In each case, a random error corresponding to a  $u'$  of 1.0 ppm was assumed (note: for the case of "perfect" data,  $u' = 0$ , no effect would be expected based on the similar finding earlier in this section for the study of the total number of equally spaced points). Figures 113 and 114 graphically present the regression results for the cases shown on page F-19. Significant variation is apparent in both figures. Whereas the distribution of random error within the given points of each case is different (thereby introducing an additional uncontrolled parameter within the study which hinders direct comparison of the results based on data spacing), it is apparent that better results (i.e., in terms of % error in  $k_0$  and  $K$ ) are obtained when the data are equally distributed throughout the entire range of interest. It should be noted that Case 1B (in Figure 113) and Case 2A (in Figure 114) yielded significantly different results from the other cases in their corresponding figures because the combination of random error and data spacing within each case caused least-squares analysis to regress a

Figure 113

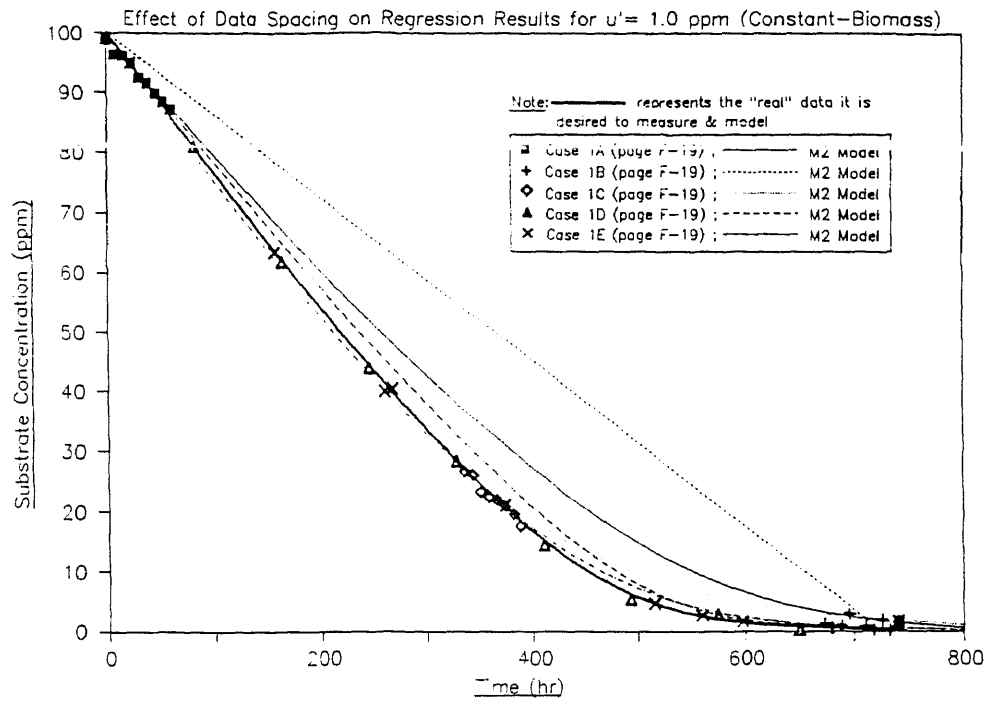
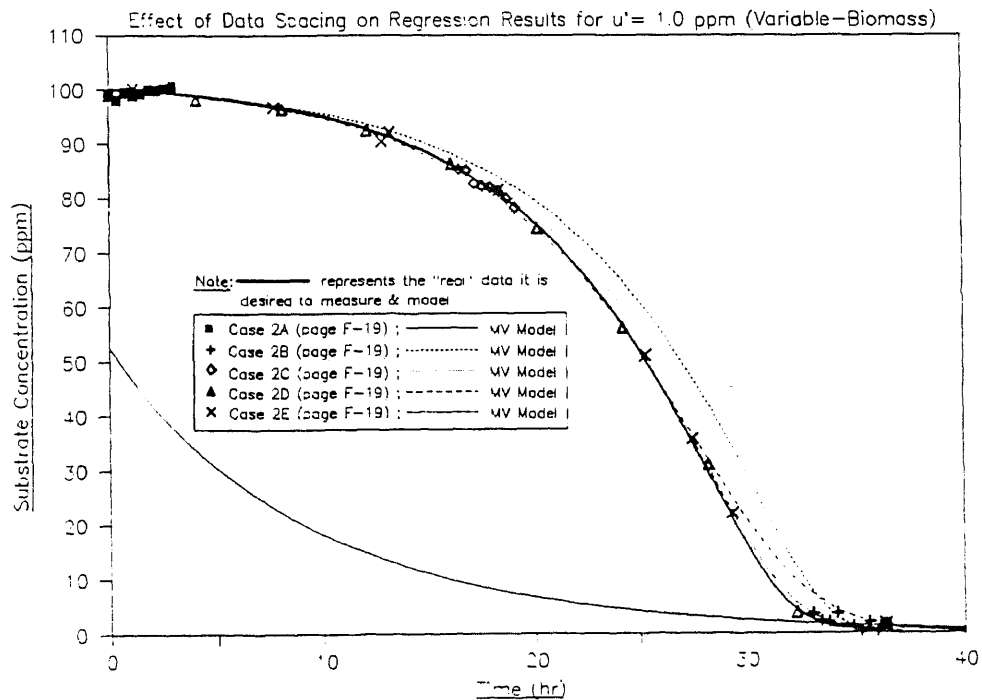


Figure 114



negative value of  $K$  and negative values of both  $k_0$  and  $K$ , respectively (note: the reasons for this are discussed in detail within Section 6).

The effect of data range truncation was evaluated for the case of constant-biomass behavior on pages F-20 through F-23 (for  $u' = 1.0$  ppm). In Experiments A through E in which the lower end of the data set is truncated progressively from 0.1 up to 25 ppm, M3 was found to be optimum (in terms of  $k_0$  and  $K$ ) for a lower  $S$  value of 10 ppm. At lower values of  $S$ , increased error was introduced into the regression analysis because of the higher inaccuracy of the corresponding  $S$  measurements (i.e., the ratio of  $u'/S$  increases as  $S$  decreases). At higher values of  $S$ , increased error was introduced into the regression analysis because of a reduction in the overall  $S$  range covered (i.e., the ratio of  $u'/(S_0-S)$  increases as  $S$  increases). Furthermore, Experiments A through E show the zero-order models to progressively improve relative to the Monod models as the lower value of  $S$  is truncated upwards. This is primarily the result of the elimination of the first-order region from the data set. Figure 115 presents a graphical comparison of the Z1 and M2 models for the  $S$  range of 100 → 25 ppm. Experiments F and G on pages F-22 and F-23 show the corresponding regression results for the  $S$  ranges from 25 ppm down to 0.1 ppm and 1.0 ppm, respectively. Both of these ranges cover the region where the transition to first-order kinetics is observed to occur. In both cases, the zero- and first-order models are statistically only a little worse than the Monod models because of the relatively large error in the data (i.e., both  $u'/S$  and  $u'/(S_0-S)$  are high). With more accurate data (i.e., lower values of  $u'$ ), the



Figure 115

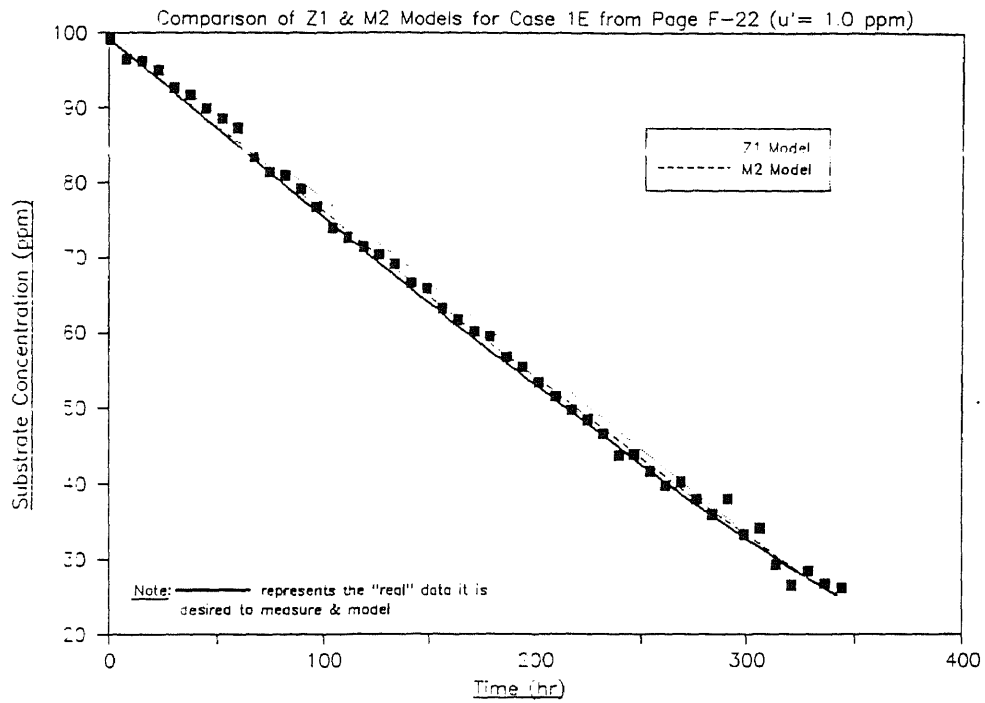
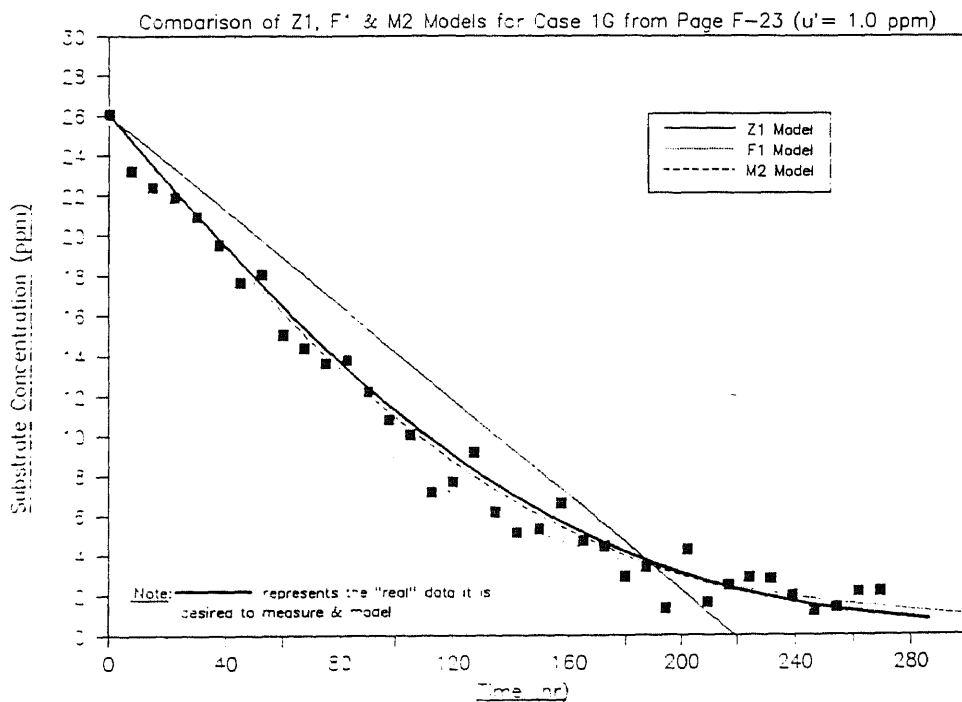


Figure 116



first-order models would be observed to perform much better than the zero-order models for the  $25 \rightarrow 0.1$  ppm S range. Figure 116 presents a graphical comparison of the M2, F1 and Z1 models for the  $25 \rightarrow 1$  ppm range.

The effect of data range truncation was evaluated for the case of variable-biomass behavior (for  $u' = 1.0$  ppm) on pages F-23 through F-25 in Experiments A through E. The MV model was found to be optimum (in terms of  $k_0$  and  $K$ ) for the S range of 100 ppm down to 1 ppm. For lower and higher final values of S, increased error was introduced into the regression analyses for the same reasons as mentioned above for the constant-biomass case. As the S range is truncated, both the ZV and FV models improve relative to the MV model. The ZV model is the better of the two because of the exclusion of the first-order effect in the data as the S range is truncated (note: the transition from zero- to first-order kinetics occurs in the 20-40 ppm range for this case). Statistically, the FV model improves relative to the MV and ZV models as the S range is truncated because of a relative decrease in the overall accuracy of the data set as reflected by an increase in  $u'/(S_0-S)$ . Figure 117 presents a graphical comparison of the MV, FV and ZV models for the  $100 \rightarrow 25$  ppm range.

Regression analysis of the  $25 \text{ ppm} \rightarrow 0.1 \text{ ppm}$  S range for the variable-biomass case was performed for all of the constant- and variable-biomass models on page F-25 in Experiment F. In general, the Monod models are best, followed by the first-order models, with the zero-order models being worst because of the data in this case being

Figure 117

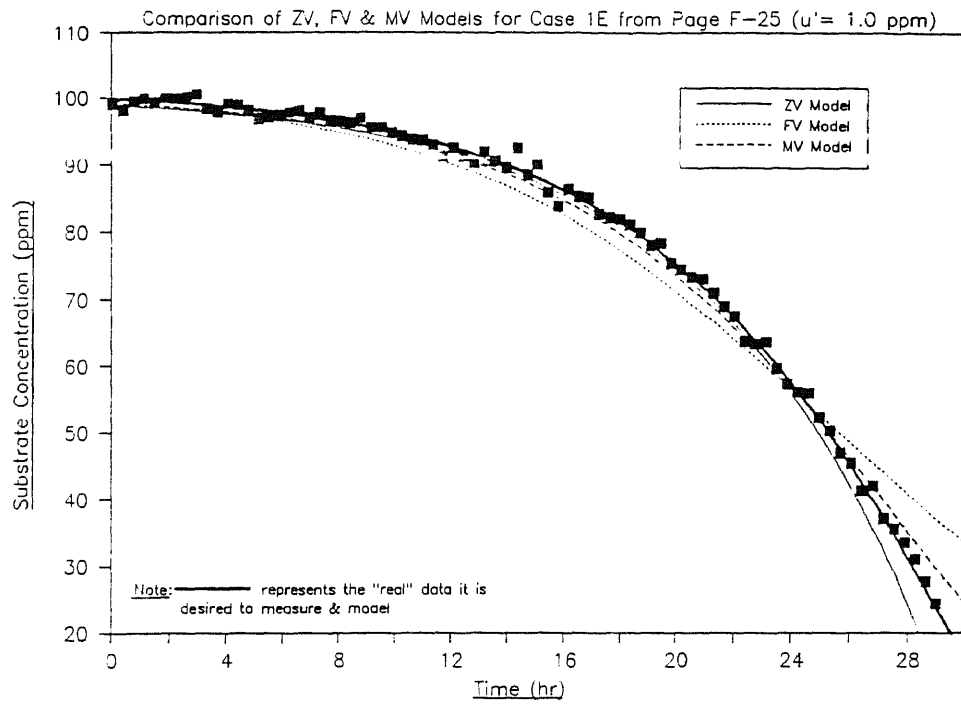
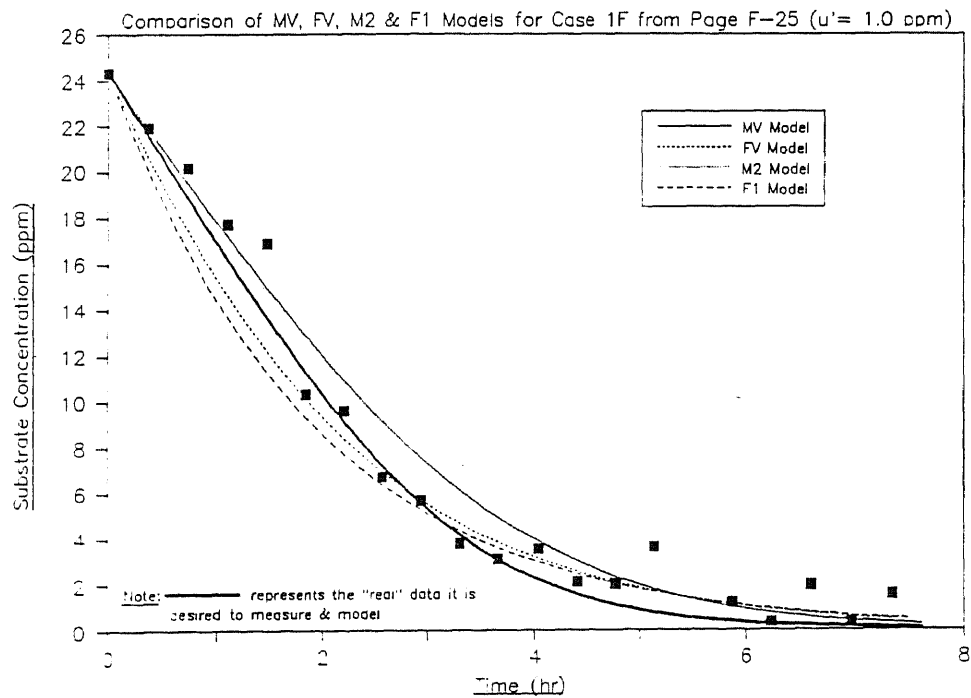


Figure 118



primarily in the first-order region. The constant- and variable-biomass models yield comparable results because the observed variable-biomass effect is relatively small (i.e.,  $B$  increases only by 32% for the  $S$  range covered). Figure 118 presents a graphical comparison of the MV, FV, M2 and F1 models for this case. While all four models are comparable for the data shown (i.e., the points which include random experimental error of magnitude  $u' = 1.0$  ppm), they all underpredict the extent of conversion relative to the "real" curve for  $S$  values below 4 ppm. This is attributed to the fact that the data points in the latter portion of the curve are, on average, higher than the "real" points because of exclusion from the regression analysis of  $S$  values equal to or less than zero. Use of arbitrarily low positive values of  $S$  (e.g.,  $S$  equal to 0.01 ppm) in place of the excluded values improves the regression results slightly, but the average value of  $S$  in the latter portion of the curve will still be higher than the "real" values as a result of the arbitrary increase in some of the randomly measured  $S$  values. This is a real concern whenever data measurements are made for  $S$  values of magnitude less than 3  $u'$ .

#### 8. Potential Benefits from Proper Model Selection

The potential benefits from proper model selection lie in the sizing of wastewater treatment reactors. An accurate model will result in the minimum reactor volume that meets design objectives. An inaccurate model will result in an inefficient design in which the reactor will either be oversized (thereby increasing capital cost) or

undersized (thereby not meeting pre-determined specifications for throughput and/or removal efficiency). The extent of oversizing or undersizing can readily be quantitated in terms of the ratio of the predicted reactor volume,  $V_p$ , to that of the theoretically minimum reactor volume,  $V_t$ , necessary to meet pre-established specifications. The ratio  $V_p/V_t$  for a CSTR is equal to the ratio of the theoretical reaction rate,  $(-r_t)$ , to the predicted reaction rate,  $(-r_p)$ . Values of  $V_p/V_t$  greater than 1 indicate oversizing while values less than 1 indicate undersizing.

A summary of analytical expressions for  $V_p/V_t$  are provided in Table 6 for a CSTR. Each expression shown refers to the volumetric inefficiency in CSTR sizing which results from the use of the indicated model instead of the theoretical or "real" model it is desired to determine. For the expressions shown, the theoretical or "real" model is assumed to be a Monod model (either M2/M3 for the case of constant-biomass behavior or MV for the case of variable-biomass behavior) with kinetic constants designated with asterisks. Examples of the effect of incorrect or inaccurate model selection on volumetric efficiency (i.e.,  $V_p/V_t$ ) in reactor design for selected cases from Section 7.2 are presented below.

Table 6

Summary of Vp/Vt Expressions for a CSTR for the Cases of  
Constant- and Variable-Biomass Behavior<sup>1</sup>

Constant-Biomass Behavior:

$$\text{Z1/Z2 Model: } (V_p/V_t) = (k^*S_e)/(k(K^*+S_e))$$

$$\text{F1/F2 Model: } (V_p/V_t) = k^*/(k(K^*+S_e))$$

$$\text{M2/M3 Model: } (V_p/V_t) = (k^*(K+S_e))/(k(K^*+S_e))$$

Variable-Biomass Behavior:

$$\text{ZV Model: } (V_p/V_t) = (k_o^*S_e)/(k_o(K^*+S_e))$$

$$\text{FV Model: } (V_p/V_t) = k_o^*/(k_o(K^*+S_e))$$

$$\text{MV Model: } (V_p/V_t) = (k_o^*(K+S_e))/(k_o(K^*+S_e))$$

$$\text{Z1/Z2 Model: } (V_p/V_t) = (k_o^*(B_i+Y_c(S_i-S_e))S_e)/(k(K^*+S_e))$$

$$\text{F1/F2 Model: } (V_p/V_t) = (k_o^*(B_i+Y_c(S_i-S_e)))/(k(K^*+S_e))$$

$$\text{M2/M3 Model: } (V_p/V_t) = (k_o^*(B_i+Y_c(S_i-S_e))(K+S_e))/(k(K^*+S_e))$$

- 1 The Vp/Vt expressions shown refer to the volumetric inefficiency in reactor sizing resulting from the use of the indicated model in place of the theoretical or "real" model it is desired to determine. The theoretical or "real" model is assumed to be a Monod model (M2/M3 for constant-biomass behavior or MV for variable-biomass behavior) with the kinetic constants designated by the asterisks.

The effect of incorrect model selection on CSTR design for the case of ideal constant-biomass behavior (i.e.,  $u'=0$ ) is demonstrated as follows in terms of  $V_p/V_t$  for the regressed models from Experiment D on page F-8 for CSTRs with  $Se$  values of 0.1 ppm:

| <u>Model</u> | <u><math>V_p/V_t</math></u> |
|--------------|-----------------------------|
| M3           | 1.000                       |
| M2           | 1.000                       |
| Z2           | 0.012                       |
| Z1           | 0.010                       |
| F2           | 1.804                       |
| F1           | 2.329                       |

The Monod models, as expected for ideal data with no experimental error, yield perfect results in terms of  $V_p/V_t$ . Use of the above incorrect zero-order models for CSTR design would result in significantly undersized vessels. The desired conversion of substrate in these vessels could only be achieved at dramatically reduced throughputs (i.e., ca. 1% of design). The above incorrect first-order models, unlike the zero-order models, result in oversized vessels. While these vessels would achieve the pre-established design specifications, it would be accomplished at a much higher capital investment than necessary. For the case of ideal constant-biomass data intermediate in order between zero and first, the zero-order models will always result in undersized vessels (i.e.,  $V_p/V_t < 1$ ) while the first-order models will always result in oversized vessels (i.e.,  $V_p/V_t > 1$ ).

The corresponding effect of incorrect model selection on CSTR design for the case of ideal variable-biomass behavior (i.e.,  $u'=0$ ) is demonstrated as follows in terms of  $V_p/V_t$  for the regressed models from Experiment D on page F-11 for CSTRs with  $Se$  values of 0.1 ppm:

| <u>Model</u> | <u><math>V_p/V_t</math></u> |
|--------------|-----------------------------|
| MV           | 1.000                       |
| M3           | -0.799                      |
| M2           | -2.169                      |
| ZV           | 0.008                       |
| Z2           | 0.031                       |
| Z1           | 0.041                       |
| FV           | 4.520                       |
| F2           | 4.363                       |
| F1           | 7.189                       |

As for the case of ideal constant-biomass data, all of the zero-order models underpredict  $V_t$ , while all of the first-order models overpredict  $V_t$ , for kinetic data of fractional order. The above M3/M2 models yield physically uninterpretable results for  $V_t$  because the regressed models from page F-11 had negative values of  $K$ . The negative values of  $V_p/V_t$  result above because the value of  $Se$  selected (i.e., 0.1 ppm) is less than the absolute values of  $K$  in both cases.



The effect of inaccuracy in regressed constants, resulting from random experimental error (i.e.,  $u'$  not equal to 0), for theoretically correct models on CSTR sizing is presented below for the cases of constant- and variable-biomass behavior from pages F-13 through F-15 and from pages F-16 and F-17, respectively:

| <u>Experiment</u> | <u><math>u'</math> (ppm)</u> | <u><math>V_p/V_t</math> for M3<br/>(p. F-13 to F-15)</u> | <u><math>V_p/V_t</math> for MV<br/>(p. F-16 and F-17)</u> |
|-------------------|------------------------------|--|---|
| -                 | 0                            | 1.000  | 1.000   |
| A                 | 0.1                          | 1.109  | 1.153   |
| B                 | 0.25                         | 1.073  | 1.255   |
| C                 | 0.5                          | 0.701  | 1.327   |
| D                 | 1.0                          | 0.435  | 1.373   |
| E                 | 2.0                          | 0.371  | 2.747   |
| F                 | 5.0                          | 0.253  | N/A   |

The above results demonstrate the importance of minimizing experimental error (i.e.,  $u'$ ) in raw kinetic data in terms of obtaining models which accurately depict reality and result in effective and cost-efficient wastewater treatment reactor designs. It should be noted that the above trends in  $V_p/V_t$  with respect to  $u'$  for both M3 and MV are the result of the particular distribution of random error evaluated in Appendix F and not any inherent characteristics of the models.

The effect of inaccuracy in regressed constants from theoretically correct models, resulting from different data sampling spacings/regularity for the case of  $u'$  equal to 1.0 ppm, on CSTR sizing is presented below for the cases of constant- and variable-biomass behavior shown previously in Figures 113 and 114, respectively:

| <u>Case</u> | <u>Description</u>     | <u>Vp/Vt for M2<br/>(refer to Fig. 113)</u> | <u>Vp/Vt for MV<br/>(refer to Fig. 114)</u> |
|-------------|------------------------|---|---|
| A           | Mostly initial points  | 1.517                                       | 10.924                                      |
| B           | Mostly final points    | -0.015                                      | 0.750                                       |
| C           | Mostly central points  | 2.227                                       | 1.603                                       |
| D           | Equally spaced points  | 0.902                                       | 1.152                                       |
| E           | Randomly spaced points | 1.439                                       | 1.844                                       |

The above tabulation clearly demonstrates that the best results are obtained when sampling is performed on a regular basis with respect to time over the entire  $S$  range of interest. Highly erroneous results can be obtained when sampling is concentrated over a time interval short enough such that  $u'$  is greater than the actual substrate converted, as demonstrated above in cases A and B. Case B for M2 and Case A for MV are especially bad because of the regression of negative rate constants for reasons stated previously in Section 7.2.

The effect of inaccuracy is regressed constants, resulting from random experimental error in  $S$  (i.e.,  $u'$ ) which approaches the absolute magnitude of  $S$ , on CSTR sizing is presented below for the models and case shown previously in Figure 118:

| <u>Model</u> | <u><math>V_p/V_t</math></u> |
|--------------|-----------------------------|
| MV           | 1.250                       |
| FV           | 1.826                       |
| M2           | 1.272                       |
| F1           | 2.096                       |

Each of the above regressed models resulted in oversizing of CSTRs because of inherent systematic error in the  $S$  data in the range where  $S$  is less than  $3u'$ . In this  $S$  range, the average value of  $S$  is inflated because of the exclusion of negative values of  $S$  which would naturally occur if the physical lower limit of 0 were not present. Whereas arbitrarily low positive values of  $S$  were used in place of  $S$  values less than or equal to 0 for the hypothetical cases evaluated in Section 7, this approach only alleviated the problem partially by lowering the average  $S$  value for the latter part of the range slightly (i.e., vs. what the average would have been if these values had been excluded entirely). Since the values which would otherwise be negative were arbitrarily increased to positive values, the average "measured"  $S$  value is naturally higher than the "real"  $S$  values it is desired to measure. The above example further demonstrates the need for controlling  $u'$  below one third of the lowest value of  $S$  of interest for design purposes in order not to regress models which result in oversized vessels.

## 9. Conclusions

Review of the open literature has demonstrated that a significant inconsistency exists with respect to the selection of kinetic expressions by authors for the modelling of raw aerobic biodegradation data. A total of 140 batch reactor biodegradation data sets extracted from the literature and previous NJIT MS theses were categorized, according to the shapes of the  $S$  vs.  $t$  curves, within the following nine biodegradation data types: (1) zero-order constant biomass, (2) first-order constant biomass, (3) Monod constant biomass, (4) Monod variable biomass, (5) first-order variable biomass, (6) zero-order variable biomass, (7) lag followed by biodegradation, (8) greater than first order, and (9) miscellaneous.

The latter two data types have no theoretical bases within biodegradation kinetics and refer to observed  $S$  vs.  $t$  curves which are more likely artifacts of the experimental methods used than intrinsic kinetic data. The common causes of data types 8 and 9 were: (i) failure to eliminate abiotic substrate removal mechanisms (e.g., adsorption, evaporation, etc.), and (ii) poor quality data (i.e., insufficient/inaccurate measurements).

The first seven data types are typical of batch reactor aerobic biodegradation data where abiotic mechanisms have been removed and mass-transfer resistances are not limiting. Furthermore, each of the first seven data types can be observed to be derived from either one or both of the two generalized biodegradation curves presented in Figure 1. While variations of the Monod model appear to be the preferred method of data analysis in most cases, this model suffers from certain problems in specific instances which hinder its universal application. Model selection recommendations given here, therefore, vary with data type. The initial critical step in the model selection procedure is the categorization of a given data set within one of the above-mentioned data types based on the shape of its  $S$  vs.  $t$  curve.

For type 1 data, the constant-biomass Monod model always yields statistically better results than the corresponding zero-order model because of the additional degree of freedom in the regression analysis provided in the Monod model by the kinetic parameter  $K$ . The Monod model, however, will regress negative values of  $K$  for type 1 data whenever the  $S$  vs.  $t$  curve can be interpreted as bending downward

(possibly as a result of random experimental error). The zero-order model is generally preferred for type 1 data, but only for application over the range of  $S$  data evaluated, since extrapolation errors can be very large.

For type 2 data, the constant-biomass Monod model will always yield statistically better results than the corresponding first-order model because of the inherent additional regressable parameter  $K$ . The Monod model, however, will regress negative values of both  $k$  and  $K$  for type 2 data whenever the  $S$  vs.  $t$  curve can be interpreted as dropping at a rate any greater than first order (possibly as a result of random experimental error). In general, the first-order model is preferred for type 2 data. It should also be noted that  $S_0$  should always be treated as a regressable parameter since it results in statistically better fits than when it is set equal to the initial substrate concentration. In this way, a given model can average out random experimental error over **all** of the data points in a given set, thereby eliminating any bias toward the first data point of a set which occurs when  $S_0$  is arbitrarily set equal to  $S$  at  $t=0$ . The logic behind the regression of  $S_0$  is that, if  $S_0$  is measured in the same way as any other value of  $S$  (e.g., by GC analysis which is the case in the data from previous NJIT MS theses), then it has no claim to an exact value.

Type 3 data are the most common for batch reactor aerobic biodegradations utilizing substrate-acclimated cultures of virtually constant biomass concentration. These data sets are of fractional order (i.e., intermediate between zero and first) and are very well represented by the constant-biomass Monod model.

The variable-biomass models reduce to the corresponding constant-biomass versions for data types 1 through 3, thereby yielding identical results in the above cases. It should be noted that the prediction of whether a given system prior to measurement will be of types 1, 2 or 3 cannot be reliably made based on knowledge of the substrate concentration range covered alone. The kinetics are determined primarily by the S/B (i.e., substrate to active biomass concentration) ratio, as well as a host of other complex environmental and metabolic factors. Determination of the S/B ratio alone is difficult due to the lack of a simple procedure by which to measure the active biomass concentration, B, accurately.

While the active biomass concentration is never truly constant due to the incessantly changing conditions within the reactor environment, data types 4 through 6 specifically refer to systems in which the active biomass concentration changes (i.e., increases) many-fold over the range of S utilized. Since biomass yield coefficients,  $Y_c$ , are low (i.e., typically between 0 and 1), the many-fold increase mentioned above will only be observed in cases where the initial active biomass concentration,  $S_0$ , is low. The main problem observed in this

thesis, for the cases where strong variable-biomass effects were evident, is that of accurately measuring  $B_0$ . All of the authors studied herein measured the total (not active) biomass concentration which did not vary proportionately with the active biomass concentration. The biomass determination methods used (e.g., dry biomass weight and absorbance) do not differentiate between substrate-specific and non-substrate specific cultures, let alone between living and dead cells of the substrate-specific culture(s). Reasonable regression results were only obtained herein for single culture (as opposed to the more common mixed culture) systems. Whereas the variable-biomass effects were still underpredicted due to overestimation of  $B_0$  because of the inability of the above methods to differentiate between living and dead cells,  $B_0$  was much less overestimated than in the mixed culture systems where non-substrate-specific cultures provided additional interferences.

The variable-biomass Monod model, MV, yields statistically better results than both the zero- and first-order variable-biomass models for all batch reactor data of types 4 through 6. While the MV model is relatively insensitive (i.e., compared to ZV and FV) to inaccuracies in biomass measurement in terms of fit (i.e.,  $\sum(t-t_{calc})^2$ ), it is very dependent on accurate  $B$  values with respect to regressing positive values for the rate constants  $k_0$  and  $K$ . MV will regress negative values of  $K$  if the value of  $B_0$  is sufficiently overestimated and it will regress negative values of both  $k_0$  and  $K$  if



$B_0$  is sufficiently underestimated. While the FV model yields positive rate constants for all values of  $B_0$  and has similar characteristics (i.e., in terms of curvature) to that of the MV model, the adequacy of fit in terms of  $\Sigma(t-t_{calc})^2$  is critically dependent on accurate  $B_0$  values. The conclusion here is that the MV model is best for data of types 4 through 6, but it requires more accurate measurement of active biomass concentration than is typically being accomplished in the literature.

Biodegradation data type 7 can be reasonably well fit by the variable-biomass models for the cases where: (i) accurate active biomass measurements are available, (ii) the lag is relatively short compared to the overall biodegradation time, and (iii) the transition from lag to biodegradation is gradual and not abrupt. The above conditions are not always met and better regression results are obtained by excluding the lag from the analysis entirely. This is the recommended approach until a better theoretical model, depicting the metabolic activities associated with the lag phase, is developed.

While many of the batch reactor aerobic biodegradation data sets evaluated in this thesis could be well represented by kinetic models, the applicability of the resulting models is limited by inadequate description of the biomass system. This limitation was demonstrated in this thesis by the regression of significantly different rate constants for purportedly identical reaction systems/conditions.

For a given model to be useful, it is necessary to know the exact conditions under which the data on which it is based was determined. Specifically, the types and concentrations of substrate-specific cultures must be known, as well as the interactive relationships between cultures and the effect of changes in the environment on their performance, in order for a given data set to be of general use for design purposes. This point cannot be underestimated. The biomass is a catalyst and needs to be defined as well as any catalyst for synthetic purposes in order for the data derived from it to be useful. This is the area where the literature and current technology is most lacking.

8 CSTR aerobic biodegradation data sets were also extracted from literature and kinetic analyses were performed on them. The quality of the data from CSTRs for modelling purposes was found to be much worse than that from batch reactors primarily due to problems associated with wall growth and the inability to readily achieve steady-state conditions. Other factors found to hinder the quality of CSTR data were: (i) most measurements were made at residence times so high that virtually complete conversion was achieved; the resulting  $S_e$  values, therefore, had relatively high experimental errors associated with them; and (ii) most of the data were for CSTRs with controlled sludging which caused the regression results to rely too heavily on

relatively inaccurate point measurements of active biomass concentration. For kinetic analysis purposes, CSTR operation as a chemostat with measurements at shorter residence times, where lower conversions occur, is recommended.

Significant variation in data quality was observed, in terms of analytical accuracy, sampling regularity and frequency, for the 148 data sets studied in this thesis. A theoretical analysis of the effect of data quality (i.e., specifically with respect to substrate concentration measurements) on regression results was, therefore, conducted for the cases of ideal constant- and variable-biomass batch reactor aerobic biodegradation data sets in order to establish some general guidelines in this area. For the case of **ideal** data (i.e., with no experimental error), no effect on the regression of rate constants for the theoretically correct Monod models is observed with variation in sampling frequency, regularity and range, providing a minimum of 4 data points exist. As random experimental error is introduced into the data sets, however, better regression results are obtained by maintaining sampling regularity and increasing sampling frequency. Random experimental error (as measured in terms of the standard deviation,  $u'$ ) should be such that  $u'$  is less than one third of the lowest value of  $S$  it is desired to measure. Otherwise, a systematic error will be introduced into the regression analysis due to the data points, on average, in the latter portion of the set where  $S$  is less than  $3 u'$ , being higher than reality because of the physical

impossibility of measuring negative values of  $S$ . Small errors in the latter portion of the set have a greater impact on the accuracy of regression results for the Monod model than comparable errors in other portions of the set because of the logarithmic functions in the linear regression analyses which inherently favor the lower values of  $S$  in terms of fit. With respect to the effects of sampling frequency, regularity and range, as well as analytical accuracy, on the fit of incorrect models (e.g., zero and first order), the only general observation that can be made is that differentiation between all models (i.e., theoretically correct and incorrect models) decreases as data quality worsens. No generalization can be made with respect to at which point the incorrect models become comparable to the correct models as a result of experimental measurement errors.

Accurate kinetic models are of importance for wastewater treatment reactor sizing. For typical biodegradation kinetics which are of fractional order, zero-order models will underpredict reactor volume (thereby failing to meet pre-established specifications for throughput and/or removal efficiency) while first-order models will overpredict reactor volume (thereby increasing the capital cost required to meet pre-established specifications). Reactor sizing, for the cases in which theoretically correct models are used, is sensitive to errors in the rate constants resulting from random experimental

error in substrate concentration measurements. Random error should be such that  $u'$  is less than one third of the lowest value of  $S$  it is desired to measure in order to yield a reliable, cost-efficient reactor design.

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## Appendix A

### Mathematical Derivation of Kinetic Expressions for the Regression of Biodegradation Rate Constants from Batch Reactor Data

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Nomenclature

a,b,c = regressable parameters

A1, A2, A3  
 B1, B2, B3  
 C1, C2, C3  
 D1, D2, D3  
 E1, E2, E3  
 F1, F2, F3  
 G1, G2, G3  
 H1, H2, H3  
 I1, I2, I3

} = variables used in matrix calculations  
(as defined on A-20 to A-22)

B = biomass concentration =  $B_0 + Y_c (S_0 - S)$

$B_0$  = initial biomass concentration

k = biodegradation rate constant =  $k_0 B$

K = constant for Monod kinetic expression

$k_0$  = biodegradation rate constant (independent of biomass concentration)

n = number of data points

r = biodegradation rate (ppm/hr)

S = substrate concentration (ppm)

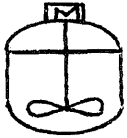
$S_0$  = initial substrate concentration (ppm)

t = time elapsed (hr)

x, y, z = variables used in regression analyses

Y = variable used in regression analyses

$Y_c$  = yield coefficient =  $(B - B_0) / (S_0 - S)$

Ideal Batch Reactor: (Performance Equation)

assume:

- i. uniform composition throughout reactor
- ii. constant reactor volume

mass balance:  $\overset{0}{\cancel{\text{input}}} = \overset{0}{\cancel{\text{output}}} + \text{disappearance} + \text{accumulation}$

$$\therefore \text{disappearance} = -\text{accumulation}$$

$$\left[ \begin{array}{l} \text{rate of loss of substrate} \\ \text{within reactor due to} \\ \text{chemical reaction} \end{array} \right] = - \left[ \begin{array}{l} \text{rate of accumulation} \\ \text{of substrate} \\ \text{within the reactor} \end{array} \right]$$

$$(-r) = -dS/dt$$

$$dt = -dS/(-r)$$

$$\int_0^t dt = - \int_{S_0}^S dS/(-r)$$

therefore,  $\boxed{t = - \int_{S_0}^S dS/(-r)}$  ; performance equation

Zero-Order Kinetics:Constant Biomass:

$$(-r) = -dS/dt = k; (k = \text{constant})$$

$$dt = -dS/k$$

$$\int_0^t dt = \int_{S_0}^S -dS/k = (-1/k) \int_{S_0}^S dS$$

$$t = (-1/k)(S-S_0) = S_0/k - S/k$$

$$\boxed{t = (-1/k)S + (S_0/k)}; \text{ (integrated zero-order kinetic expression for constant biomass)}$$

the rate constant,  $k$ , can be regressed from experimental  $S$  vs.  $t$  data using the method of least-squares analysis; regression can be performed with respect to  $S$  or  $t$ , since the above integrated expression is explicit in both; for the purpose of this study regression is performed with respect to  $t$

One-Parameter: (regress for  $k$  only; let  $S_0$  assume the experimental value of  $S$  at  $t = 0$ )

$$\begin{aligned} t &= (-1/k)S + (S_0/k) \\ &= (1/k)(S_0 - S) \end{aligned}$$

let,  $y = t$ ; (experimental data)  
 $x = (S_0 - S)$ ; (experimental data)  
 $a = (1/k) = \text{slope}$ ; (regressable parameter)

therefore,  $y = ax$

by least-squares analysis (refer to A-17)

$$a = \Sigma xy / \Sigma x^2 = (1/k)$$

$$\boxed{k = (1/a) = \Sigma x^2 / \Sigma xy}$$

Two-Parameter: (regress for both k and So)

$$t = (-1/k)S + (So/k)$$

let,  $y = t$ ; (experimental data)

$x = S$ ; (experimental data)

$a = (-1/k) = \text{slope}$ ; (regressable parameter)

$b = (So/k) = \text{intercept}$ ; (regressable parameter)

therefore,  $y = ax + b$

by least-squares analysis (refer to A-18)

$$a = (n \sum xy - \sum x \sum y) / (n \sum x^2 - (\sum x)^2)$$

$$b = (\sum x^2 \sum y - \sum xy \sum x) / (n \sum x^2 - (\sum x)^2)$$

$$k = (-1/a) = (n \sum x^2 - (\sum x)^2) / (\sum x \sum y - n \sum xy)$$

$$So = (-b/a) = (\sum x^2 \sum y - \sum xy \sum x) / (\sum x \sum y - n \sum xy)$$

calculation of S as a function of t is straightforward (once the regressable parameters have been determined) for either the one- or two-parameter models since the integrated zero-order kinetic expression is explicit with respect to S:

$$S = So - kt$$

Zero-Order Kinetics:Variable Biomass:

$$\begin{aligned}
 (-r) &= -dS/dt = k; \quad k = f(\text{biomass concentration}) \\
 &= k_o B \\
 &= k_o (B_o + Y_c(S_o - S))
 \end{aligned}$$

where,

$B_o, S_o, Y_c$  = constants (assumed available)

$k_o$  = regressable parameter

$$\begin{aligned}
 -dS/dt &= k_o (B_o + Y_c(S_o - S)) \\
 -k_o dt &= dS/(B_o + Y_c(S_o - S)) = dS/(B_o + Y_c S_o - Y_c S)
 \end{aligned}$$

$$\begin{aligned}
 \int_0^t -k_o dt &= -k_o t = \int_{S_o}^S dS/(B_o + Y_c S_o - Y_c S) \\
 &= (-1/Y_c) \int_{S_o}^S (-Y_c dS)/(B_o + Y_c S_o - Y_c S) \\
 &= (-1/Y_c) \ln(B_o + Y_c S_o - Y_c S) \Big|_{S_o}^S \\
 &= (-1/Y_c) (\ln(B_o + Y_c S_o - Y_c S) - \ln(B_o + Y_c S_o - Y_c S_o)) \\
 &= (-1/Y_c) (\ln(B_o + Y_c S_o - Y_c S) - \ln(B_o))
 \end{aligned}$$

$$\boxed{t = (1/k_o Y_c) (\ln(B_o + Y_c S_o - Y_c S) - \ln(B_o))}; \quad (\text{integrated zero-order kinetic expression for variable biomass})$$

the rate constant,  $k_o$ , can be regressed from experimental  $S$  vs.  $t$  data, provided biomass data are available, using the method of least-squares analysis; regression is performed with respect to the explicit variable  $t$

One-Parameter: (regress for  $k_o$  only;  $B_o, S_o$ , and  $Y_c$  are assumed given)

$$\begin{aligned}
 t &= (1/k_o Y_c) (\ln(B_o + Y_c S_o - Y_c S) - \ln(B_o)) \\
 &= (1/k_o Y_c) (\ln((B_o + Y_c S_o - Y_c S)/B_o))
 \end{aligned}$$

$$\begin{aligned}
 \text{let, } y &= t; \quad (\text{experimental data}) \\
 x &= \ln((B_o + Y_c S_o - Y_c S)/B_o); \quad (\text{experimental data}) \\
 a &= (1/k_o Y_c) = \text{slope}; \quad (\text{regressable parameter})
 \end{aligned}$$

therefore,  $y = ax$

by least-squares analysis (refer to A-17)

$$a = \Sigma xy / \Sigma x^2 = (1/k_o Y_c)$$

$$\boxed{k_o = (1/a Y_c) = \Sigma x^2 / (Y_c \Sigma xy)}$$

calculation of S as a function of t is straightforward once  $k_o$  has been determined since the integrated zero-order kinetic expression for variable biomass is explicit with respect to S:

$$S = (B_o + Y_c S_o - B_o \exp(-k_o Y_c t)) / Y_c$$

First-Order Kinetics:Constant Biomass:

$$(-r) = -dS/dt = kS; (k = \text{constant})$$

$$dt = -dS/(kS)$$

$$\int_0^t dt = \int_{S_0}^S -dS/(kS) = (-1/k) \int_{S_0}^S dS/S$$

$$t = (-1/k) \ln(S/S_0) \quad ; (\text{integrated first-order kinetic expression for constant biomass})$$

the rate constant,  $k$ , can be regressed from experimental  $S$  vs.  $t$  data using the method of least-squares analysis; regression is performed with respect to the explicit variable  $t$

One-Parameter: (regress for  $k$  only; let  $S_0$  assume the experimental value of  $S$  at  $t=0$ )

$$t = (-1/k) \ln(S/S_0) \\ = (1/k) \ln(S_0/S)$$

let,  $y = t$ ; (experimental data)  
 $x = \ln(S_0/S)$ ; (experimental data)  
 $a = (1/k) = \text{slope}$ ; (regressable parameter)  
 therefore,  $y = ax$

by least-squares analysis (refer to A-17)

$$a = \sum xy / \sum x^2 = (1/k)$$

$$k = (1/a) = \sum x^2 / \sum xy$$

Two-Parameter: (regress for both k and So)

$$\begin{aligned} t &= (-1/k) \ln(S/S_o) \\ &= (1/k) \ln(S_o/S) \\ &= (1/k) (\ln S_o - \ln S) \\ &= (-1/k) \ln S + ((\ln S_o)/k) \end{aligned}$$

let,  $y = t$ ; (experimental data)  
 $x = \ln S$ ; (experimental data)  
 $a = (-1/k) = \text{slope}$ ; (regressable parameter)  
 $b = (\ln S_o)/k = \text{intercept}$ ; (regressable parameter)

therefore,  $y = ax + b$

by least-squares analysis (refer to A-18)

$$a = (n \sum xy - \sum x \sum y) / (n \sum x^2 - (\sum x)^2)$$

$$b = (\sum x^2 \sum y - \sum xy \sum x) / (n \sum x^2 - (\sum x)^2)$$

$$k = (-1/a) = (n \sum x^2 - (\sum x)^2) / (\sum x \sum y - n \sum xy)$$

$$S_o = \exp(-b/a) = \exp((\sum x^2 \sum y - \sum xy \sum x) / (\sum x \sum y - n \sum xy))$$

calculation of S as a function of t is straightforward (once the regressable parameters have been determined) for either the one- or two-parameter models since the integrated first-order kinetic expression for constant biomass is explicit with respect to S:

$$S = S_o * \exp(-kt)$$



First-Order Kinetics:Variable Biomass:

$$\begin{aligned}
 (-r) &= -dS/dt = kS; \quad k = f(\text{biomass concentration}) \\
 &= k_o B \\
 &= k_o (B_o + Y_c(S_o - S))
 \end{aligned}$$

where,

$B_o, S_o, Y_c$  = constants (assumed available)

$k_o$  = regressable parameter

$$-dS/dt = k_o (B_o + Y_c(S_o - S))S$$

$$-k_o dt = dS / ((B_o + Y_c(S_o - S))S)$$

$$\begin{aligned}
 \int_0^t -k_o dt &= -k_o t = \int_{S_o}^S dS / ((B_o + Y_c(S_o - S))S) \\
 &= \int_{S_o}^S dS / ((B_o + Y_c S_o - Y_c S)S) \\
 &= (-1 / (B_o + Y_c S_o)) \ln((B_o + Y_c S_o - Y_c S) / S) \Big|_{S_o}^S \\
 &= (-1 / (B_o + Y_c S_o)) (\ln((B_o + Y_c S_o - Y_c S) / S) \\
 &\quad - \ln((B_o + Y_c S_o - Y_c S_o) / S_o)) \\
 &= (-1 / (B_o + Y_c S_o)) (\ln((B_o + Y_c S_o - Y_c S) / S) \\
 &\quad - \ln(B_o / S_o)) \\
 &= (-1 / (B_o + Y_c S_o)) \ln((B_o + Y_c S_o - Y_c S) S_o / (B_o S))
 \end{aligned}$$

$$t = (-1 / (k_o (B_o + Y_c S_o))) \ln((B_o S) / ((B_o + Y_c S_o - Y_c S) S_o)) ;$$

(integrated first-order kinetic expression for variable biomass)

the rate constant,  $k_o$ , can be regressed from experimental  $S$  vs.  $t$  data, provided biomass data are available, using the method of least-squares analysis; regression is performed with respect to the explicit variable  $t$

One-Parameter: (regress for  $k_o$  only;  $B_o, S_o$ , and  $Y_c$  are assumed given)

$$t = (-1 / (k_o (B_o + Y_c S_o))) \ln(B_o S / ((B_o + Y_c S_o - Y_c S) S_o))$$

let,  $y = t$ ; (experimental data)

$x = \ln(B_o S / ((B_o + Y_c S_o - Y_c S) S_o))$ ; (experimental data)

$a = (-1 / (k_o (B_o + Y_c S_o)))$  = slope; (regressable parameter)

therefore,  $y = ax$

by least-squares analysis (refer to A-17)

$$a = \sum xy / \sum x^2 = (-1 / (k_o(Bo + YcSo)))$$

$$k_o = (-1 / (a(Bo + YcSo))) = - \sum x^2 / (\sum xy(Bo + YcSo))$$

calculation of S as a function of t is straightforward once  $k_o$  has been determined since the integrated first-order kinetic expression for variable biomass is explicit with respect to S:

$$S = (Bo + YcSo) / (Yc + (Bo/So) \exp((Bo + YcSo)k_o t))$$

Monod Kinetics:Constant Biomass:

$$(-r) = -dS/dt = kS/(K+S); \text{ (k and K are constants)}$$

$$dt = -(K+S)dS/Sk$$

$$\begin{aligned} \int_0^t k dt &= \int_{S_0}^S -(K+S)dS/S = \int_{S_0}^S -(K/S)dS - \int_{S_0}^S dS \\ &= -K \int_{S_0}^S dS/S - \int_{S_0}^S dS \\ &= -K \ln S \Big|_{S_0}^S - S \Big|_{S_0}^S \\ &= -K \ln(S/S_0) - (S-S_0) \end{aligned}$$

$$t = (K/k) \ln(S_0/S) + (1/k)(S_0 - S); \text{ (integrated Monod kinetic expression for constant biomass)}$$

the rate constants (k and K) can be regressed from experimental S vs. t data using the method of least-squares analysis; regression is performed with respect to the explicit variable t

Two-Parameter: (regress for k and K only; let  $S_0$  assume the experimental value of S at t = 0)

$$t = (K/k) \ln(S_0/S) + (1/k)(S_0 - S)$$

$$\begin{aligned} \text{let, } y &= t; \text{ (experimental data)} \\ x &= \ln(S_0/S); \text{ (experimental data)} \\ z &= (S_0 - S); \text{ (experimental data)} \\ a &= (K/k); \text{ (regressable parameter)} \\ b &= (1/k); \text{ (regressable parameter)} \end{aligned}$$

$$\text{therefore, } y = ax + bz$$

by least-squares analysis (refer to A-19)

$$\begin{aligned} a &= (\sum xy \sum z^2 - \sum xz \sum yz) / (\sum x^2 \sum z^2 - (\sum xz)^2) \\ &= (K/k) \end{aligned}$$

$$\begin{aligned} b &= (\sum yz \sum x^2 - \sum xy \sum xz) / (\sum x^2 \sum z^2 - (\sum xz)^2) \\ &= (1/k) \end{aligned}$$

$$k = (1/b) = (\sum x^2 \sum z^2 - (\sum xz)^2) / (\sum yz \sum x^2 - \sum xy \sum xz)$$

$$K = (a/b) = (\sum xy \sum z^2 - \sum xz \sum yz) / (\sum yz \sum x^2 - \sum xy \sum xz)$$

Three-Parameter: (regress for k, K and So)

$$\begin{aligned} t &= (K/k)\ln(So/S) + (1/k)(So-S) \\ &= (K/k)\ln So - (K/k)\ln S + (So/k) - (S/k) \\ &= (-K/k)\ln S + (-1/k)S + ((K/k)\ln So + (So/k)) \end{aligned}$$

let,  $y = t$ ; (experimental data)  
 $x = \ln S$ ; (experimental data)  
 $z = S$ ; (experimental data)  
 $a = (-K/k)$ ; (regressable parameter)  
 $b = (-1/k)$ ; (regressable parameter)  
 $c = ((K/k)\ln So + (So/k))$ ; (regressable parameter)

therefore,  $y = ax + bz + c$

by least-squares analysis (refer to A-20)

$$\begin{aligned} a &= (-K/k); \text{ (see A-22)} \\ b &= (-1/k); \text{ (see A-22)} \\ c &= (K/k)\ln So + (So/k); \text{ (see A-22)} \end{aligned}$$

$$k = (-1/b); \text{ (see A-22)}$$

$$K = (a/b); \text{ (see A-22)}$$

So, or S for any value of t for either the two- or three-parameter models can be determined by a trial-and-error procedure such as Newton's Rule (refer to A-23) provided the values of k and K are known; straightforward calculation of S is not possible since the integrated Monod expressions are not explicit with respect to S.

Monod Kinetics:Variable Biomass:

$$(-r) = -dS/dt = kS/(K + S); \quad K = \text{constant}$$

$$k = f(\text{biomass concentration})$$

$$= k_o B$$

$$= k_o (B_o + Y_c(S_o - S))$$

where,

$B_o, S_o, Y_c = \text{constants (assumed available)}$   
 $k_o, K = \text{regressable parameters}$

$$-dS/dt = k_o (B_o + Y_c(S_o - S)) S / (K + S)$$

$$-k_o dt = (K + S) dS / (S(B_o + Y_c(S_o - S)))$$

$$\begin{aligned} \int_0^t -k_o dt &= -k_o t = \int_{S_o}^S (K + S) dS / (S(B_o + Y_c S_o - Y_c S)) \\ &= K \int_{S_o}^S dS / ((B_o + Y_c S_o - Y_c S) S) + \\ &\quad \int_{S_o}^S dS / (B_o + Y_c S_o - Y_c S) \\ &= (-K / (B_o + Y_c S_o)) \ln((B_o + Y_c S_o - Y_c S) / S) \Big|_{S_o}^S + \\ &\quad (-1 / Y_c) \ln(B_o + Y_c S_o - Y_c S) \Big|_{S_o}^S \\ &= (-K / (B_o + Y_c S_o)) \ln((B_o + Y_c S_o - Y_c S) / S) - \\ &\quad (-K / (B_o + Y_c S_o)) \ln((B_o + Y_c S_o - Y_c S_o) / S_o) + \\ &\quad (-1 / Y_c) \ln(B_o + Y_c S_o - Y_c S) - \\ &\quad (-1 / Y_c) \ln(B_o + Y_c S_o - Y_c S_o) \\ &= (-K / (B_o + Y_c S_o)) \ln((B_o + Y_c S_o - Y_c S) S_o / (B_o S)) \\ &\quad + (-1 / Y_c) \ln((B_o + Y_c S_o - Y_c S) / B_o) \end{aligned}$$

|  |
|--|
| $t = \left( \frac{K}{k_o (B_o + Y_c S_o)} \right) \ln \left( \frac{(B_o + Y_c S_o - Y_c S) S_o}{(B_o S)} \right) + \left( \frac{1}{k_o Y_c} \right) \ln \left( \frac{(B_o + Y_c S_o - Y_c S)}{B_o} \right);$ |
|--|

Monod kinetic expression for variable biomass)

the rate constants,  $k_o$  and  $K$ , can be regressed from experimental  $S$  vs.  $t$  data, provided biomass data are available, using the method of least-squares analysis; regression is performed with respect to the explicit variable  $t$

Two-Parameter: (regress for  $k_o$  and  $K$ ;  $B_o$ ,  $Y_c$  and  $S_o$  are assumed given)

$$t = (K/(k_o(B_o + Y_c S_o))) \ln((B_o + Y_c S_o - Y_c S)/B_o) + (1/(k_o Y_c)) \ln((B_o + Y_c S_o - Y_c S)/B_o)$$

let,  $y = t$ ; (experimental data)

$$x = \ln((B_o + Y_c S_o - Y_c S)/B_o); \text{ (experimental data)}$$

$$z = \ln((B_o + Y_c S_o - Y_c S)/B_o); \text{ (experimental data)}$$

$$a = (K/(k_o(B_o + Y_c S_o))); \text{ (regressable parameter)}$$

$$b = (1/(k_o Y_c)); \text{ (regressable parameter)}$$

therefore,  $y = ax + bz$

by least-square analysis (refer to A-19)

$$a = (\sum xy \sum z^2 - \sum xz \sum yz) / (\sum x^2 \sum z^2 - (\sum xz)^2) \\ = (K/(k_o(B_o + Y_c S_o)))$$

$$b = (\sum yz \sum x^2 - \sum xy \sum xz) / (\sum x^2 \sum z^2 - (\sum xz)^2) \\ = (1/(k_o Y_c))$$

$$k_o = (1/b Y_c) \\ = (\sum x^2 \sum z^2 - (\sum xz)^2) / (Y_c (\sum yz \sum x^2 - \sum xy \sum xz))$$

$$K = (a(B_o + Y_c S_o)) / (b Y_c) \\ = ((\sum xy \sum z^2 - \sum xz \sum yz)(B_o + Y_c S_o)) / ((\sum yz \sum x^2 - \sum xy \sum xz) Y_c)$$

calculation of  $S$  as a function of  $t$  can be determined by a trial-and-error procedure (once the regressable parameters have been determined) such as Newton's Rule (refer to A-23); straight-forward calculation of  $S$  is not possible since the integrated Monod expression for variable biomass is not explicit with respect to  $S$

Method of Least-Squares Analysis: DerivationsCase 1:  $Y = ax$ 

given a set of data (i.e.,  $y$  as a function of  $x$ ) it can be fit to an algebraic expression  
 $Y = ax$

let,  $E = \text{error}$

$$= y - Y = y - (ax) = y - ax$$

"a" should be chosen such that the sum of the square of the error,  $\sum E^2$  (or  $f(a)$ ), is minimized

$$f(a) = \sum E^2 = \sum (y - ax)^2$$

$$df(a)/da = d(\sum (y - ax)^2)/da$$

$$= 2\sum (y - ax)(-x)$$

$$= 0$$

$$\text{therefore, } \sum xy - a\sum x^2 = 0; \quad \boxed{a = \sum xy / \sum x^2}$$

Case 2:  $Y = ax + b$

given a set of data (i.e.,  $y$  as a function of  $x$ ), it can be fit to an algebraic expression  $Y = ax + b$

let,  $E = \text{error}$

$$= y - Y = y - (ax + b) = y - ax - b$$

"a" and "b" should be chosen such that the sum of the square of the error,  $\sum E^2$  (or  $f(a, b)$ ), is minimized

$$f(a, b) = \sum E^2 = \sum (y - ax - b)^2$$

$$\begin{aligned} \partial f(a, b) / \partial a &= \partial / \partial a (\sum (y - ax - b)^2) \\ &= 2 \sum (y - ax - b)(-x) \\ &= 0 \end{aligned}$$

$$\begin{aligned} \partial f(a, b) / \partial b &= \partial / \partial b (\sum (y - ax - b)^2) \\ &= 2 \sum (y - ax - b)(-1) \\ &= 0 \end{aligned}$$

$$\begin{aligned} \text{therefore, } \sum xy - a \sum x^2 - b \sum x &= 0 \\ \sum y - a \sum x - nb &= 0; \\ (n = \# \text{ of data points}) \end{aligned}$$

simultaneous solution of the above two equations for the two unknowns (i.e.,  $a$  and  $b$ ) algebraically yields:

$$a = (n \sum xy - \sum x \sum y) / (n \sum x^2 - (\sum x)^2)$$

$$b = (\sum x^2 \sum y - \sum xy \sum x) / (n \sum x^2 - (\sum x)^2)$$



Case 3:  $Y = ax + bz$

given a set of data (i.e.,  $y$  as a function of  $x$  and  $z$ ), it can be fit to an algebraic expression  $Y = ax + bz$

let,  $E = \text{error}$

$$= y - Y = y - (ax + bz) = y - ax - bz$$

"a" and "b" should be chosen such that the sum of the square of the error,  $\sum E^2$  (or  $f(a,b)$ ), is minimized

$$f(a,b) = \sum E^2 = \sum (y - ax - bz)^2$$

$$\begin{aligned} \partial f(a,b)/\partial a &= \partial/\partial a (\sum (y - ax - bz)^2) \\ &= 2 \sum (y - ax - bz)(-x) \\ &= 0 \end{aligned}$$

$$\begin{aligned} \partial f(a,b)/\partial b &= \partial/\partial b (\sum (y - ax - bz)^2) \\ &= 2 \sum (y - ax - bz)(-z) \\ &= 0 \end{aligned}$$

$$\begin{aligned} \text{therefore, } \sum xy - a \sum x^2 - b \sum xz &= 0 \\ \sum yz - a \sum xz - b \sum z^2 &= 0 \end{aligned}$$

simultaneous solution of the above two equations for the two unknowns (i.e.,  $a$  and  $b$ ) algebraically yields:

$$a = (\sum xy \sum z^2 - \sum yz \sum xz) / (\sum x^2 \sum z^2 - (\sum xz)^2)$$

$$b = (\sum yz \sum x^2 - \sum xy \sum xz) / (\sum x^2 \sum z^2 - (\sum xz)^2)$$

Case 4:  $Y = ax + bz + c$

given a set of data (i.e.,  $y$  as a function of  $x$  and  $z$ ), it can be fit to an algebraic expression  $Y = ax + bz + c$

let,  $E = \text{error}$

$$= y - Y = y - (ax + bz + c)$$

$$= y - ax - bz - c$$

"a", "b", and "c" should be chosen such that the sum of the square of the error,  $\sum E^2$  (or  $f(a,b,c)$ ) is minimized

$$f(a,b,c) = \sum E^2 = \sum (y - ax - bz - c)^2$$

$$\begin{aligned} \partial f(a,b,c) / \partial a &= \partial / \partial a (\sum (y - ax - bz - c)^2) \\ &= 2 \sum (y - ax - bz - c) (-x) \\ &= 0 \end{aligned}$$

$$\begin{aligned} \partial f(a,b,c) / \partial b &= \partial / \partial b (\sum (y - ax - bz - c)^2) \\ &= 2 \sum (y - ax - bz - c) (-z) \\ &= 0 \end{aligned}$$

$$\begin{aligned} \partial f(a,b,c) / \partial c &= \partial / \partial c (\sum (y - ax - bz - c)^2) \\ &= 2 \sum (y - ax - bz - c) (-1) \\ &= 0 \end{aligned}$$

$$\begin{aligned} \text{therefore, } \sum xy - a \sum x^2 - b \sum xz - c \sum x &= 0 \\ \sum yz - a \sum xz - b \sum z^2 - c \sum z &= 0 \\ \sum y - a \sum x - b \sum z - nc &= 0 \\ (n = \# \text{ of data points}) \end{aligned}$$

simultaneous solution of the above three equations for the three unknowns (i.e.,  $a$ ,  $b$ , and  $c$ ) can be accomplished using matrix algebra

rewrite the above equations,

$$\begin{aligned} (\sum x^2) a + (\sum xz) b + (\sum x) c &= \sum xy \\ (\sum xz) a + (\sum z^2) b + (\sum z) c &= \sum yz \\ (\sum x) a + (\sum z) b + (n) c &= \sum y \end{aligned}$$

redefine the equations,

$$\begin{aligned} (A1) \quad a + (B1) b + (C1) c &= D1 \\ (A2) \quad a + (B2) b + (C2) c &= D2 \\ (A3) \quad a + (B3) b + (C3) c &= D3 \end{aligned}$$

where,

$$\begin{aligned} A1 &= \sum x^2; & B1 &= \sum xz; & C1 &= \sum x; & D1 &= \sum xy \\ A2 &= \sum xz; & B2 &= \sum z^2; & C2 &= \sum z; & D2 &= \sum yz \\ A3 &= \sum x; & B3 &= \sum z; & C3 &= n; & D3 &= \sum y \end{aligned}$$

therefore the matrix can be written:

$$\begin{bmatrix} A1 & B1 & C1 & | & D1 \\ A2 & B2 & C2 & | & D2 \\ A3 & B3 & C3 & | & D3 \end{bmatrix}$$

divide row 1 by A1, row 2 by A2, and row 3 by A3,

$$\begin{bmatrix} 1 & B1/A1 & C1/A1 & | & D1/A1 \\ 1 & B2/A2 & C2/A2 & | & D2/A2 \\ 1 & B3/A3 & C3/A3 & | & D3/A3 \end{bmatrix}$$

subtract row 1 from both rows 2 and 3,

$$\begin{bmatrix} 1 & B1/A1 & C1/A1 & | & D1/A1 \\ 0 & B2/A2 - B1/A1 & C2/A2 - C1/A1 & | & D2/A2 - D1/A1 \\ 0 & B3/A3 - B1/A1 & C3/A3 - C1/A1 & | & D3/A3 - D1/A1 \end{bmatrix}$$

rewrite the above matrix,

$$\begin{bmatrix} 1 & E1 & F1 & | & G1 \\ 0 & E2 & F2 & | & G2 \\ 0 & E3 & F3 & | & G3 \end{bmatrix}$$

$$\begin{aligned} \text{where, } E1 &= B1/A1 & ; & F1 = C1/A1 & ; & G1 = D1/A1 \\ E2 &= B2/A2 - E1 & ; & F2 = C2/A2 - F1 & ; & G2 = D2/A2 - G1 \\ E3 &= B3/A3 - E1 & ; & F3 = C3/A3 - F1 & ; & G3 = D3/A3 - G1 \end{aligned}$$

divide row 2 by E2 and row 3 by E3,

$$\begin{bmatrix} 1 & E1 & F1 & | & G1 \\ 0 & 1 & F2/E2 & | & G2/E2 \\ 0 & 1 & F3/E3 & | & G3/E3 \end{bmatrix}$$

subtract row 2 multiplied by  $E1$  from row 1; subtract row 2, as is, from row 3,

$$\begin{bmatrix} 1 & 0 & F1 - F2*(E1/E2) & | & G1 - G2*(E1/E2) \\ 0 & 1 & F2/E2 & | & G2/E2 \\ 0 & 0 & F3/E3 - F2/E2 & | & G3/E3 - G2/E2 \end{bmatrix}$$

rewrite the above matrix,

$$\begin{bmatrix} 1 & 0 & H1 & | & I1 \\ 0 & 1 & H2 & | & I2 \\ 0 & 0 & H3 & | & I3 \end{bmatrix}$$

$$\begin{aligned} \text{where, } H1 &= F1 - E1 * H2; & I1 &= G1 - E1 * I2 \\ H2 &= F2/E2 & ; & I2 = G2/E2 \\ H3 &= F3/E3 - H2 & ; & I3 = G3/E3 - I2 \end{aligned}$$

divide row 3 by  $H3$ ,

$$\begin{bmatrix} 1 & 0 & H1 & | & I1 \\ 0 & 1 & H2 & | & I2 \\ 0 & 0 & 1 & | & I3/H3 \end{bmatrix}$$

subtract row 3, multiplied by  $H1$ , from row 1;  
subtract row 3, multiplied by  $H2$ , from row 2,

$$\begin{bmatrix} 1 & 0 & 0 & | & I1 - H1 * I3/H3 \\ 0 & 1 & 0 & | & I2 - H2 * I3/H3 \\ 0 & 0 & 1 & | & I3/H3 \end{bmatrix}$$

$$\text{therefore, } \begin{cases} a = I1 - I3 * H1/H3 \\ b = I2 - I3 * H2/H3 \\ c = I3/H3 \end{cases}$$

$$\begin{aligned} \text{where, } H1 &= F1 - E1 * H2; & I1 &= G1 - E1 * I2 \\ H2 &= F2/E2 & ; & I2 = G2/E2 \\ H3 &= F3/E3 - H2 & ; & I3 = G3/E3 - I2 \end{aligned}$$

$$\begin{aligned} \text{where, } E1 &= B1/A1 & ; & F1 = C1/A1 & ; & G1 = D1/A1 \\ E2 &= B2/A2 - E1; & F2 &= C2/A2 - F1; & G2 &= D2/A2 - G1 \\ E3 &= B3/A3 - E1; & F3 &= C3/A3 - F1; & G3 &= D3/A3 - G1 \end{aligned}$$

$$\begin{aligned} \text{where, } A1 &= \sum x^2; & B1 &= \sum xz & ; & C1 = \sum x; & D1 &= \sum xy \\ A2 &= \sum xz; & B2 &= \sum z^2 & ; & C2 = \sum z; & D2 &= \sum yz \\ A3 &= \sum x; & B3 &= \sum z & ; & C3 = n; & D3 &= \sum y \end{aligned}$$

Newton's Rule:

This technique is used for finding a root of a single-variable non-linear equation, such as any of the following three forms of the integrated Monod kinetics:

- (1a):  $t = (K/k)\ln(S_0/S) + (1/k)(S_0 - S)$ ; constant biomass (2-parameter)  
 $= a \ln(S_0/S) + b (S_0 - S)$ ; (refer to A-13)
- (2a):  $t = (-K/k)\ln S + (-1/k)S + ((K/k)\ln S_0 + S_0/k)$ ; constant biomass (3-par.)  
 $= a \ln S + b S + c$ ; (refer to A-14)
- (3a):  $t = (K/(k_0(B_0 + Y_c S_0)))\ln((B_0 + Y_c S_0 - Y_c S)S_0/(B_0 S)) + (1/(k_0 Y_c))\ln((B_0 + Y_c S_0 - Y_c S)/B_0)$ ; variable biomass (2-parameter)  
 $= a \ln((B_0 + Y_c S_0 - Y_c S)S_0/(B_0 S)) + b \ln((B_0 + Y_c S_0 - Y_c S)/B_0)$ ;  
 (refer to A-16)

Rewrite each expression as a function of S equal to zero:

- (1b):  $f(S) = a \ln(S/S_0) + b(S - S_0) + t = 0$
- (2b):  $f(S) = a \ln S + b S + c - t = 0$
- (3b):  $f(S) = a \ln((B_0 + Y_c S_0 - Y_c S)S_0/(B_0 S)) + b \ln((B_0 + Y_c S_0 - Y_c S)/B_0) - t = 0$

For the above three expressions, a, b, c,  $S_0$ ,  $B_0$  and  $Y_c$  are assumed given while S is to be determined for various values of t.

The first derivatives of each of the above three expressions are:

- (1c):  $f'(S) = a/S + b = 0$
- (2c):  $f'(S) = a/S + b = 0$
- (3c):  $f'(S) = -(a+b)Y_c/(B_0 + Y_c S_0 - Y_c S) - a/S = 0$

The solution of S for a given t may be multiple (i.e., more than one root). To get the desired root requires a good initial guess of S-- $S_0$  is usually a good value to use. Once the initial value of S is chosen, an iterative procedure is used to calculate subsequent values of S until the difference between the new and old value is negligible. For this study, the convergence value (i.e., new value minus old value) was arbitrarily chosen to be 0.0001.

```

Let,  $S_i = S_o$ 
 $S_{i+1} = S_i - f(S_i)/f'(S_i)$ 
if  $|S_{i+1} - S_i| < 0.0001$ ,  $S = S_{i+1}$ !
if not, let  $S_i = S_{i+1}$  and repeat the above calculations until
the convergence value is attained

```

For the purpose of this study, a simple program was written in BASIC for the SHARP PC-1500 pocket computer to calculate  $S$  for various values of  $t$ . This program is listed below:

```

5:  S = 0 : SN = 0 : T = 0 : FS = 0 : FPS = 0
10:  A2 = 0 : B2 = 0 : S0 = 0
15:  A3 = 0 : B3 = 0 : C3 = 0
20:  AV = 0 : BV = 0 : B0 = 0 : YC = 0
25:  INPUT "a(2-parameter; constant) =", A2
30:  INPUT "b(2-parameter; constant) =", B2
35:  INPUT "So = ", S0
40:  INPUT "a(3-parameter; constant) =", A3
45:  INPUT "b(3-parameter; constant) =", B3
50:  INPUT "c(3-parameter; constant) =", C3
55:  INPUT "a(2-parameter; variable) =", AV
60:  INPUT "b(2-parameter; variable) =", BV
65:  INPUT "Bo =", B0
70:  INPUT "Yc =", YC
75:  S = S0
80:  FS = A2*LN(S/S0)+B2*(S-S0)+T
85:  FPS = A2/S + B2
90:  SN = S - FS/FPS
95:  IF ABS (SN-S)<1E-4 THEN GOTO 110
100: S = SN
105: GOTO 80
110: PRINT "MONOD 2-PARAMETER (CONST)"
115: PRINT "t = "; T; "; S = "; SN
120: IF T = 6 THEN GOTO 135
125: T = T + 0.25
130: GOTO 100
135: T = 0
140: S = S0
145: FS = A3*LNS + B3*S+C3-T
150: FPS = A3/S + B3
155: SN = S - FS/FPS
160: IF ABS(SN - S)<1E-4 THEN GOTO 175
165: S = SN
170: GOTO 145
175: PRINT "MONOD 3-PARAMETER (CONST)"
180: PRINT "t = "; T; "; S = "; SN
185: IF T = 6 THEN GOTO 200
190: T = T + 0.25
195: GOTO 165

```

```

200: T = 0
205: S = SO
210: FS = AV*LN((BO+YC*SO-YC*S)*SO/(BO*S))
      + BV*LN((BO+YC*SO-YC*S)/BO)-T
215: FPS = -(AV+BV)*YC/(BO+YC*SO-YC*S)-AV/S
220: SN = S - FS/FPS
225: IF ABS(SN-S)<1E-4 THEN GOTO 240
230: S = SN
235: GOTO 210
240: PRINT "MONOD 2-PARAMETER (VAR)"
245: PRINT "t = "; T; "; S = "; SN
250: IF T = 6 THEN GOTO 265
255: T = T + 0.25
260: GOTO 230
265: END

```

The above program requires that the results from the regression analyses for each form of Monod equation be inputted upon request of the pocket computer (as specified by the program):

```

2-parameter model (constant biomass)→a,b,So
3-parameter model (constant biomass)→a,b,c
2-parameter model (variable biomass)→a,b,Eo,Yc

```

The program will calculate values of S for corresponding values of t from 0 to 6 hours in 1/4-hour increments for the 2-parameter constant biomass model first, then the 3-parameter model, and then finally the 2-parameter variable-biomass model. The units for S in this study are parts per million (ppm).

To calculate S for a single value of t, rather than the above range, modify the above program as indicated below. Insert the following program statement:

```

76: INPUT "t=", T

```

Delete the following program statements: 120, 125, 130, 135, 140, 185, 190, 195, 200, 205, 250, 255, 260.

To calculate S for multiple values of t without reinputting the regressed results every time, insert the following program statement:

```

264: GOTO 76

```

The last modification will require the program to be manually terminated once all the desired results are attained, since an infinite loop exists.

## Appendix B

Mathematical Derivation of Kinetic Expressions for  
the Regression of Biodegradation Rate Constants  
from Continuous Stirred-Tank Reactor Data (i.e., CSTR)



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Nomenclature

a,b,c = regressable parameters

A,B,C = miscellaneous variables (as defined on B-10 and B-14)

Be = biomass concentration =  $B_i + Y_c(S_i - S_e)$

Bi = initial biomass concentration

k = biodegradation rate constant =  $k_o B_e$

K = constant for Monod kinetic expression

$k_o$  = biodegradation rate constant (independent of biomass concentration)

Q = volumetric flow rate

Qe = effluent volumetric flow rate

Qi = inlet volumetric flow rate

(-r) = biodegradation rate (ppm/hr.)

Se = effluent substrate concentration (ppm)

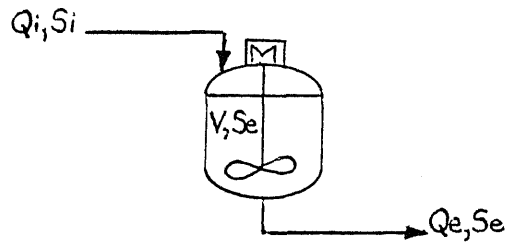
Si = feed substrate concentration (ppm)

V = reactor volume

x,y,z = variables used in regression analyses

$Y_c$  = yield coefficient =  $(B_e - B_i)/(S_i - S_e)$

$\tau = (V/Q)$  = reactor time constant

Ideal Continuous Stirred-Tank Reactor: (Performance Eqn.)

assume:

- i. steady state
- ii. uniform composition throughout reactor
- iii. constant reactor volume

mass balance: input = output + disappearance + accumulation<sup>0</sup>  
 input-output = disappearance by reaction

$$Q_i S_i - Q_e S_e = (-r)V$$

$$(S_i - S_e)/(-r) = V/Q ; (Q_i = Q_e = Q)$$

therefore,  $\tau = (V/Q) = (S_i - S_e)/(-r)$ ; performance equation

Zero-Order Kinetics:Constant Biomass:

$$(-r) = (S_i - S_e)/\tau = k ; (k = \text{constant})$$

$$(S_i - S_e) = k\tau$$

$$\tau = (-1/k)S_e + (S_i/k) ; (\text{zero-order kinetic expression for constant biomass})$$

the rate constant,  $k$ , can be regressed from experimental  $S_e$  vs.  $\tau$  (i.e.,  $V/Q$ ) data using the method of least-squares analysis; regression can be performed with respect to  $S_e$  or  $\tau$  since the above expression is explicit in both; for the purpose of this study, regression is performed with respect to  $\tau$

One-Parameter: (regress for  $k$  only; let  $S_i$  assume the experimental value of the feed substrate concentration)

$$\tau = (S_i - S_e)/k$$

$$\tau = (1/k)(S_i - S_e)$$

let,  $y = \tau = (V/Q)$  ; (experimental data)  
 $x = (S_i - S_e)$  ; (experimental data)  
 $a = (1/k) = \text{slope}$  ; (regressable parameter)

therefore,  $y = ax$

by least-squares analysis (refer to A-17)

$$a = \sum xy / \sum x^2 = (1/k)$$

$$k = (1/a) = \sum x^2 / \sum xy$$

Two-Parameter: (regress for  $k$  and  $S_i$ ; this is applicable only for data where the actual feed substrate concentration is held constant--otherwise, the one-parameter model must be used)

$$\tau = (-1/k)Se + (Si/k)$$

let,  $y = \tau = (V/Q)$  ; (experimental data)

$x = Se$  ; (experimental data)

$a = (-1/k) = \text{slope}$  ; (regressable parameter)

$b = (Si/k) = \text{intercept}$  ; (regressable parameter)

therefore,  $y = ax + b$

by least-squares analysis (refer to A-18)

$$a = (n\sum xy - \sum x \sum y) / (n\sum x^2 - (\sum x)^2)$$

$$b = (\sum x^2 \sum y - \sum xy \sum x) / (n\sum x^2 - (\sum x)^2)$$

$$k = (-1/a) = (n\sum x^2 - (\sum x)^2) / (\sum x \sum y - n\sum xy)$$

$$Si = (-b/a) = (\sum x^2 \sum y - \sum xy \sum x) / (\sum x \sum y - n\sum xy)$$

calculation of  $Se$  as a function of  $\tau$  is straightforward (once the regressable parameters have been determined) for either the one- or two-parameter models since the zero-order kinetic expression is explicit with respect to  $Se$ :

$$Se = Si - k\tau$$

Zero-Order Kinetics:Variable Biomass:

$$(-r) = (S_i - S_e)/\tau = k ; k = f(\text{biomass concentration})$$

$$= k_o B_e$$

$$= k_o (B_i + Y_c(S_i - S_e))$$

where,

$B_i, S_i, Y_c$  = constants  
(assumed available)

$k_o$  = regressable  
parameter

$$(-r) = (S_i - S_e)/\tau = k_o (B_i + Y_c(S_i - S_e))$$

$$\tau = (S_i - S_e) / (k_o (B_i + Y_c(S_i - S_e))) ; \text{ (zero-order kinetic expression for variable biomass)}$$

the rate constant,  $k_o$ , can be regressed from experimental  $S_e$  vs.  $\tau$  (i.e.,  $V/Q$ ) data using the method of least-squares analysis, provided biomass data are available; regression is performed with respect to the explicit variable  $\tau$

One-Parameter: (regress for  $k_o$  only;  $B_i, S_i$ , and  $Y_c$  are assumed given)

$$\tau = (1/k_o) ((S_i - S_e) / (B_i + Y_c(S_i - S_e)))$$

where,

$y = (V/Q)$  ; (experimental data)

$x = (S_i - S_e) / (B_i + Y_c(S_i - S_e))$  ; (experimental data)

$a = (1/k_o)$  = slope ; (regressable parameter)

therefore,  $y = ax$

by least-squares analysis (refer to A-17)

$$a = \sum xy / \sum x^2 = (1/k_o)$$

$$k_o = (1/a) = \sum x^2 / \sum xy$$

calculation of  $S_e$  as a function of  $\tau$  is straightforward once  $k_o$  has been determined since the zero-order kinetic expression for variable biomass is explicit with respect to  $S_e$ :

$$S_e = S_i - (k_o \tau B_i) / (1 - k_o \tau Y_c)$$

First-Order Kinetics:Constant Biomass:

$$(-r) = (S_i - S_e)/\tau = kS_e ; (k = \text{constant})$$

$$(S_i - S_e)/S_e = k\tau$$

$$\tau = (1/k)((S_i - S_e)/S_e) ; (\text{first-order kinetic expression for constant biomass})$$

the rate constant,  $k$ , can be regressed from experimental  $S_e$  vs.  $\tau$  (i.e.,  $V/Q$ ) data using the method of least-squares analysis; regression is performed with respect to the explicit variable  $\tau$

One-Parameter: (regress for  $k$  only; let  $S_i$  assume the experimental value of the feed substrate concentration)

$$\tau = (1/k)((S_i - S_e)/S_e)$$

let,

$$\begin{aligned} y &= \tau = (V/Q) ; (\text{experimental data}) \\ x &= ((S_i - S_e)/S_e) ; (\text{experimental data}) \\ a &= (1/k) = \text{slope} ; (\text{regressable parameter}) \end{aligned}$$

therefore,  $y = ax$

by least-squares analysis (refer to A-17)

$$a = \sum xy / \sum x^2 = (1/k)$$

$$k = (1/a) = \sum x^2 / \sum xy$$

Two-Parameter: (regress for  $k$  and  $S_i$ ; this is applicable only for data where the actual feed substrate concentration is held constant--otherwise, the one-parameter model must be used)

$$\begin{aligned} \tau &= (1/k)((S_i - S_e)/S_e) \\ &= (1/k)((S_i/S_e) - 1) \\ &= (S_i/k)(1/S_e) + (-1/k) \end{aligned}$$

let,

$y = \gamma = (V/Q)$  ; (experimental data)  
 $x = (1/Se)$  ; (experimental data)  
 $a = (Si/k) = \text{slope}$  ; (regressable parameter)  
 $b = (-1/k) = \text{intercept}$  ; (regressable parameter)

therefore,  $y = ax + b$

by least-squares analysis (refer to A-18)

$a = (Si/k) = (n \sum xy - \sum x \sum y) / (n \sum x^2 - (\sum x)^2)$   
 $b = (-1/k) = (\sum x^2 \sum y - \sum xy \sum x) / (n \sum x^2 - (\sum x)^2)$

$$k = (-1/b) = (n \sum x^2 - (\sum x)^2) / (\sum xy \sum x - \sum x^2 \sum y)$$

$$Si = (-a/b) = (n \sum xy - \sum x \sum y) / (\sum xy \sum x - \sum x^2 \sum y)$$

calculation of Se as a function of  $\gamma$  is straightforward (once the regressable parameters have been determined) for either the one- or two-parameter models since the first-order kinetic expression is explicit with respect to Se:

$$Se = Si / (1 + k \gamma)$$



First-Order Kinetics:Variable Biomass:

$$(-r) = (S_i - S_e) / \tau = k S_e ; k = f(\text{biomass concentration})$$

$$= k_o B_e$$

$$= k_o (B_i + Y_c (S_i - S_e))$$

where,

$B_i, S_i, Y_c = \text{constants}$   
(assumed available)

$k_o = \text{regressable parameter}$

$$(-r) = (S_i - S_e) / \tau = k_o (B_i + Y_c (S_i - S_e)) S_e$$

$$\tau = (1/k_o) ((S_i - S_e) / ((B_i + Y_c (S_i - S_e)) S_e)) ; \text{ (first-order kinetic expression for variable biomass)}$$

the rate constant,  $k_o$ , can be regressed from experimental  $S_e$  vs.  $\tau$  (i.e.,  $V/Q$ ) data using the method of least-squares analysis, provided biomass data are available; regression is performed with respect to the explicit variable  $\tau$

One-Parameter: (regress for  $k_o$  only;  $B_i, S_i$  and  $Y_c$  are assumed given)

$$\tau = (1/k_o) ((S_i - S_e) / ((B_i + Y_c (S_i - S_e)) S_e))$$

let,

$$y = \tau = (V/Q) ; \text{ (experimental data)}$$

$$x = (S_i - S_e) / ((B_i + Y_c (S_i - S_e)) S_e) ; \text{ (experimental data)}$$

$$a = (1/k_o) = \text{slope} ; \text{ (regressable parameter)}$$

therefore,  $y = ax$ 

by least-squares analysis (refer to A-17)

$$a = (1/k_o) = \sum xy / \sum x^2$$

$$k_o = (1/a) = \sum x^2 / \sum xy$$

the first-order kinetic expression for variable biomass is a linear 2nd-order polynomial with respect to  $S_e$ ; as such, the calculation of  $S_e$  as a function of  $\tau$  can be accomplished (providing  $k_o$  has been determined) by using the quadratic formula:

$$S_e^2 (Y_c k_o \tau) + S_e (-1 - Y_c S_i k_o \tau - B_i k_o \tau) + (S_i) = 0$$

where,  $A = (Y_c k_o \tau)$  $B = (-1 - Y_c S_i k_o \tau - B_i k_o \tau)$  $C = (S_i)$ 

$$\text{therefore, } S_e = \frac{-B \pm (B^2 - 4AC)^{0.5}}{(2A)}$$

Monod Kinetics:Constant Biomass:

$$(-r) = (S_i - S_e)/\tau = kS_e/(K + S_e) ; (k \text{ and } K \text{ are constants})$$

$$\tau = (S_i - S_e)(K + S_e)/(kS_e)$$

$$\tau = ((S_i - S_e)(K + S_e))/(kS_e) ; (\text{Monod kinetic expression for constant biomass})$$

the rate constants (k and K) can be regressed from experimental  $S_e$  vs.  $\tau$  (i.e.,  $V/Q$ ) data using the method of least-squares analysis; regression is performed with respect to the explicit variable  $\tau$

Two-Parameter: (regress for k and K only; let  $S_i$  assume the experimental value of the feed substrate concentration)

$$\begin{aligned}\tau &= ((S_i - S_e)(K + S_e))/(kS_e) \\ &= (S_i - S_e)K/(kS_e) + (S_i - S_e)S_e/(kS_e) \\ &= (K/k)((S_i - S_e)/S_e) + (1/k)(S_i - S_e)\end{aligned}$$

let,

$$\begin{aligned}y &= \tau = (V/Q) ; (\text{experimental data}) \\ x &= ((S_i - S_e)/S_e) ; (\text{experimental data}) \\ z &= (S_i - S_e) ; (\text{experimental data}) \\ a &= (K/k) ; (\text{regressable parameter}) \\ b &= (1/k) ; (\text{regressable parameter})\end{aligned}$$

therefore,  $y = ax + bz$

by least-squares analysis (refer to A-19)

$$\begin{aligned}a &= (K/k) = (\sum xy \sum z^2 - \sum yz \sum xz) / (\sum x^2 \sum z^2 - (\sum xz)^2) \\ b &= (1/k) = (\sum yz \sum x^2 - \sum xy \sum xz) / (\sum x^2 \sum z^2 - (\sum xz)^2)\end{aligned}$$

$$k = (1/b) = (\sum x^2 \sum z^2 - (\sum xz)^2) / (\sum yz \sum x^2 - \sum xy \sum xz)$$

$$K = (a/b) = (\sum xy \sum z^2 - \sum yz \sum xz) / (\sum yz \sum x^2 - \sum xy \sum xz)$$

Three-Parameter: (regress for k, K and Si; this is applicable only for data where the actual feed substrate concentration is held constant--otherwise the two-parameter model must be used)

$$\begin{aligned}\tau &= ((Si-Se)(K + Se))/(kSe) \\ &= (SiK + (Si-K)Se - Se^2)/(kSe) \\ &= (SiK/k)(1/Se) + (Si-K)/k - (1/k)Se \\ &= (SiK/k)(1/Se) + (-1/k) Se + ((Si-K)/k)\end{aligned}$$

let,  
 $y = \tau = (V/Q)$  ; (experimental data)  
 $x = (1/Se)$  ; (experimental data)  
 $z = Se$  ; (experimental data)  
 $a = (SiK/k)$  ; (regressable parameter)  
 $b = (-1/k)$  ; (regressable parameter)  
 $c = ((Si-K)/k)$  ; (regressable parameter)

therefore,  $y = ax + bz + c$

by least-squares analysis (refer to A-20)

$a = (SiK/k)$  ; (see A-22)  
 $b = (-1/k)$  ; (see A-22)  
 $c = ((Si-K)/k)$  ; (see A-22)

$$k = (-1/b) ; \text{ (see A-22)}$$

$$K = (c + (c^2 - 4ba)^{0.5})/(2b) ; \text{ (see A-22)}$$

$$Si = (-c + (c^2 - 4ba)^{0.5})/(2b) ; \text{ (see A-22)}$$

the Monod kinetic expression for constant biomass is a linear 2nd-order polynomial with respect to Se; as such, the calculation of Se as a function of  $\tau$  can be accomplished (once the regressable parameters have been determined) by using the quadratic formula:

$$Se = \frac{-(k\tau + K - Si) \pm ((k\tau + K - Si)^2 + 4SiK)^{0.5}}{2}$$

Monod Kinetics:Variable Biomass:

$$(-r) = (Si-Se)/\tau = kSe/(K + Se) ; k = \begin{matrix} \text{f(biomass con-} \\ \text{centration)} \\ = koBe \\ = ko(Bi + Yc(Si-Se)) \end{matrix}$$

where,  
Bi, Si, Yc = constants  
(assumed available)  
ko = regressable  
parameter

$$(-r) = (Si-Se)/\tau = ko(Bi + Yc(Si-Se))Se/(K + Se)$$

$$\tau = (1/ko)(Si-Se)(K + Se)/((Bi + Yc(Si-Se))Se) ; \text{(Monod kinetic expression for variable biomass)}$$

the rate constants (ko and K) can be regressed from experimental Se vs.  $\tau$  (i.e., V/Q) data using the method of least-squares analysis, provided biomass data are available; regression is performed with respect to the explicit variable  $\tau$

Two-Parameter: (regress for ko and K only; Bi, Si and Yc are assumed given)

$$\tau = (K/ko)((Si-Se)/((Bi+Yc(Si-Se))Se)) + (1/ko)((Si-Se)/(Bi + Yc(Si - Se)))$$

let,

$$\begin{aligned} y &= \tau = (V/Q); \text{(experimental data)} \\ x &= ((Si-Se)/((Bi + Yc(Si-Se))Se)) ; \text{(experimental data)} \\ z &= ((Si-Se)/(Bi + Yc(Si-Se))) ; \text{(experimental data)} \\ a &= (K/ko) ; \text{(regressable parameter)} \\ b &= (1/ko) ; \text{(regressable parameter)} \end{aligned}$$

therefore,  $y = ax + bz$

by least-squares analysis (refer to A-19)

$$a = (K/k_o) = (\sum xy \sum z^2 - \sum yz \sum xz) / (\sum x^2 \sum z^2 - (\sum xz)^2)$$

$$b = (1/k_o) = (\sum yz \sum x^2 - \sum xy \sum xz) / (\sum x^2 \sum z^2 - (\sum xz)^2)$$

$$k_o = (1/b) = (\sum x^2 \sum z^2 - (\sum xz)^2) / (\sum yz \sum x^2 - \sum xy \sum xz)$$

$$K = (a/b) = (\sum xy \sum z^2 - \sum yz \sum xz) / (\sum yz \sum x^2 - \sum xy \sum xz)$$

the Monod kinetic expression for variable biomass is a linear 2nd-order polynomial with respect to  $S_e$ ; as such, the calculation of  $S_e$  as a function of  $\tau$  can be accomplished (once the regressable parameters have been determined) by using the quadratic formula:

$$S_e^2 (1 - k_o Y_c \tau) + S_e (B k_o \tau + Y_c S i k_o \tau + K - S i) + (-S i K) = 0$$

$$\text{let, } A = (1 - k_o Y_c \tau)$$

$$B = (B k_o \tau + Y_c S i k_o \tau + K - S i)$$

$$C = (-S i K)$$

$$\text{therefore, } S_e = \frac{-B + (B^2 - 4AC)^{0.5}}{(2A)}$$

Appendix C

Sample Hand Calculations and LOTUS 123 Spreadsheets  
for the Regression of Batch Reactor Data

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Sample Hand CalculationsBatch Reactor Data Analysis:

Raw Data\* -  $B_0 = 19.3$  ppm\*\*  
 $Y_c = 0.136$

| <u>t(hr)</u> | <u>S(ppm)</u> |
|--------------|---------------|
| 0            | 160           |
| 1            | 150           |
| 9            | 140           |
| 12           | 110           |
| 13           | 80            |
| 15           | 90            |
| 19           | 20            |
| 28           | 10            |

\* Literature reference: Klecka, G.M., et al. (refer to page D-4).

\*\*Refer to A-3 for clarification of nomenclature.



Zero-Order Kinetics (Constant Biomass)

One-Parameter Model:  $t = (1/k)(S_0 - S)$  ; (refer to A-5)  
 $y = a \quad x$

| <u>y=t</u> | <u>x=S<sub>0</sub>-S</u> | <u>xy</u>     | <u>x<sup>2</sup></u> | <u>yc=tc=ax</u> | <u>(t-tc)<sup>2</sup></u> | <u>Sc = S<sub>0</sub>-kt</u> |
|------------|--------------------------|---------------|----------------------|-----------------|---------------------------|------------------------------|
| 0          | 0                        | 0             | 0                    | 0               | 0                         | 160                          |
| 1          | 10                       | 10            | 100                  | 1.7             | 0.49                      | 154                          |
| 9          | 20                       | 180           | 400                  | 3.5             | 30.25                     | 108                          |
| 12         | 50                       | 600           | 2500                 | 8.6             | 11.56                     | 91                           |
| 13         | 80                       | 1040          | 6400                 | 13.8            | 0.64                      | 85                           |
| 15         | 70                       | 1050          | 4900                 | 12.1            | 8.41                      | 73                           |
| 19         | 140                      | 2660          | 19600                | 24.2            | 27.04                     | 50                           |
| 28         | 150                      | <u>4200</u>   | <u>22500</u>         | 25.9            | <u>4.41</u>               | -2                           |
|            |                          | $\Sigma=9740$ | $\Sigma=56400$       |                 | $\Sigma=82.80$            |                              |

$$a = \Sigma xy / \Sigma x^2 = 9740 / 56400 = 0.1727 \text{ hr/ppm}$$

$$k = (1/a) = 5.79 \text{ ppm/hr}$$

Zero-Order Kinetics (Constant Biomass)

Two-Parameter Model:  $t = (-1/k)S + (S_0/k)$  ; (refer to A-6)  
 $y = \frac{1}{a} x + \frac{b}{a}$

| <u>y=t</u>  | <u>x=S</u>   | <u>xy</u>     | <u>x<sup>2</sup></u> | <u>yc=tc=ax+b</u> | <u>(t-tc)<sup>2</sup></u> | <u>Sc = S<sub>0</sub>-kt</u> |
|-------------|--------------|---------------|----------------------|-------------------|---------------------------|------------------------------|
| 0           | 160          | 0             | 25600                | 2.2               | 4.84                      | 175                          |
| 1           | 150          | 150           | 22500                | 3.8               | 7.84                      | 168                          |
| 9           | 140          | 1260          | 19600                | 5.3               | 13.69                     | 116                          |
| 12          | 110          | 1320          | 12100                | 9.8               | 4.84                      | 96                           |
| 13          | 80           | 1040          | 6400                 | 14.4              | 1.96                      | 89                           |
| 15          | 90           | 1350          | 8100                 | 12.9              | 4.41                      | 76                           |
| 19          | 20           | 380           | 400                  | 23.5              | 20.25                     | 50                           |
| <u>28</u>   | <u>10</u>    | <u>280</u>    | <u>100</u>           | 25.0              | <u>9.00</u>               | -9                           |
| $\Sigma=97$ | $\Sigma=760$ | $\Sigma=5780$ | $\Sigma=94800$       |                   | $\Sigma=66.83$            |                              |

$$a = (n\Sigma xy - \Sigma x \Sigma y) / (n\Sigma x^2 - (\Sigma x)^2)$$

$$= (8(5780) - (760)(97)) / (8(94800) - (760)^2)$$

$$= -0.1520 \text{ hr./ppm}$$

$$b = (\Sigma x^2 \Sigma y - \Sigma xy \Sigma x) / (n\Sigma x^2 - (\Sigma x)^2)$$

$$= ((94800)(97) - (5780)(760)) / (8(94800) - (760)^2)$$

$$= 26.564 \text{ hr.}$$

$$k = (-1/a) = 6.579 \text{ ppm/hr.}$$

$$S_0 = (-b/a) = 174.8 \text{ ppm}$$

First-Order Kinetics (Constant Biomass)

One-Parameter Model:  $t = (1/k) \ln(S_0/S)$  ; (refer to A-9)  
 $y = a \quad x$

| <u>y=t</u> | <u>x=ln(S<sub>0</sub>/S)</u> | <u>xy</u>       | <u>x<sup>2</sup></u> | <u>yc=tc=ax</u> | <u>(t-tc)<sup>2</sup></u> | <u>Sc = f(t)*</u> |
|------------|------------------------------|-----------------|----------------------|-----------------|---------------------------|-------------------|
| 0          | 0                            | 0               | 0                    | 0               | 0                         | 160               |
| 1          | 0.0645                       | 0.0645          | 0.0042               | 0.7             | 0.09                      | 146               |
| 9          | 0.1335                       | 1.2015          | 0.0178               | 1.4             | 57.76                     | 70                |
| 12         | 0.3747                       | 4.4964          | 0.1404               | 4.1             | 62.41                     | 53                |
| 13         | 0.6931                       | 9.0103          | 0.4804               | 7.5             | 30.25                     | 48                |
| 15         | 0.5754                       | 8.6310          | 0.3311               | 6.2             | 77.44                     | 40                |
| 19         | 2.0794                       | 39.5094         | 4.3239               | 22.5            | 12.25                     | 28                |
| 28         | 2.7726                       | <u>77.6325</u>  | <u>7.6873</u>        | 30.0            | <u>4.00</u>               | 12                |
|            |                              | $\Sigma=140.55$ | $\Sigma=12.985$      |                 | $\Sigma=244.20$           |                   |

$$a = \Sigma xy / \Sigma x^2 = 140.55 / 12.985 = 10.82 \text{ hr.}$$

$$k = (1/a) = 0.0924/\text{hr.}$$

$$* Sc = S_0 \cdot \exp(-kt)$$

First-Order Kinetics (Constant Biomass)Two-Parameter Model:  $t = (-1/k) \ln S + ((\ln S_0)/k)$ ; (refer to A-10)

$$y = a \quad x + b$$

| <u>y=t</u>  | <u>x=lnS</u>    | <u>xy</u>       | <u>x^2</u>      | <u>yc=tc=ax+b</u> | <u>(t-tc)^2</u> | <u>Sc = f(t)*</u> |
|-------------|-----------------|-----------------|-----------------|-------------------|-----------------|-------------------|
| 0           | 5.0752          | 0               | 25.758          | 5.4               | 29.16           | 313               |
| 1           | 5.0106          | 5.011           | 25.106          | 5.9               | 24.01           | 276               |
| 9           | 4.9416          | 44.474          | 24.419          | 6.5               | 6.25            | 102               |
| 12          | 4.7005          | 56.406          | 22.095          | 8.4               | 12.96           | 71                |
| 13          | 4.3820          | 56.966          | 19.202          | 11.0              | 4.00            | 62                |
| 15          | 4.4998          | 67.497          | 20.248          | 10.0              | 25.00           | 49                |
| 19          | 2.9957          | 56.918          | 8.974           | 22.1              | 9.61            | 30                |
| <u>28</u>   | <u>2.3026</u>   | <u>64.473</u>   | <u>5.302</u>    | 27.7              | <u>0.09</u>     | 10                |
| $\Sigma=97$ | $\Sigma=33.908$ | $\Sigma=351.75$ | $\Sigma=151.10$ |                   | $\Sigma=111.08$ |                   |

$$a = (n \Sigma xy - \Sigma x \Sigma y) / (n \Sigma x^2 - (\Sigma x)^2)$$

$$= ((8)(351.75) - (33.908)(97)) / ((8)(151.1) - (33.908)^2)$$

$$= -8.0457$$

$$b = (\Sigma x^2 \Sigma y - \Sigma xy \Sigma x) / (n \Sigma x^2 - (\Sigma x)^2)$$

$$= ((151.1)(97) - (351.75)(33.908)) / ((8)(151.1) - (33.908)^2)$$

$$= 46.227$$

$$k = (-1/a) = 0.124/\text{hr.}$$

$$S_0 = \exp(-b/a) = 313 \text{ ppm}$$

$$* S_c = S_0 \exp(-kt)$$

Monod Kinetics (Constant Biomass)

Two-Parameter Model:  $t = (K/k)\ln(S_0/S) + (1/k)(S_0 - S)$  ; (refer to A-13)  
 $y = a \quad x \quad + \quad b \quad z$

| <u>y=t</u> | <u>x=ln(S<sub>0</sub>/S)</u> | <u>z = (S<sub>0</sub>-S)</u> | <u>xy</u>       | <u>xz</u>       | <u>yz</u>     | <u>x<sup>2</sup></u> | <u>z<sup>2</sup></u> |
|------------|------------------------------|------------------------------|-----------------|-----------------|---------------|----------------------|----------------------|
| 0          | 0                            | 0                            | 0               | 0               | 0             | 0                    | 0                    |
| 1          | 0.0645                       | 10                           | 0.0645          | 0.645           | 10            | 0.0042               | 100                  |
| 9          | 0.1335                       | 20                           | 1.2015          | 2.670           | 180           | 0.0178               | 400                  |
| 12         | 0.3747                       | 50                           | 4.4964          | 18.735          | 600           | 0.1404               | 2500                 |
| 13         | 0.6931                       | 80                           | 9.0103          | 55.448          | 1040          | 0.4804               | 6400                 |
| 15         | 0.5754                       | 70                           | 8.6310          | 40.278          | 1050          | 0.3311               | 4900                 |
| 19         | 2.0794                       | 140                          | 39.5094         | 291.116         | 2660          | 4.3239               | 19600                |
| 28         | 2.7726                       | 150                          | <u>77.6325</u>  | <u>415.890</u>  | <u>4200</u>   | <u>7.6873</u>        | <u>22500</u>         |
|            |                              |                              | $\Sigma=140.55$ | $\Sigma=824.78$ | $\Sigma=9740$ | $\Sigma=12.985$      | $\Sigma=56400$       |

$$a = (\Sigma xy \Sigma z^2 - \Sigma xz \Sigma yz) / (\Sigma x^2 \Sigma z^2 - (\Sigma xz)^2)$$

$$= ((140.55)(56400) - (824.78)(9740)) / ((12.985)(56400) - (824.78)^2)$$

$$= -2.041$$

$$b = (\Sigma yz \Sigma x^2 - \Sigma xy \Sigma xz) / (\Sigma x^2 \Sigma z^2 - (\Sigma xz)^2)$$

$$= ((9740)(12.985) - (140.55)(824.78)) / ((12.985)(56400) - (824.78)^2)$$

$$= 0.20255$$

$$k = (1/b) = (1/0.20255) = 4.94 \text{ ppm/hr.}$$

$$K = (a/b) = (-2.041/0.20255) = -10.1 \text{ ppm}$$

| $y_c = t_c = ax + bz$ | $(t - t_c)^2$                | $Sc^*$ |
|-----------------------|------------------------------|--------|
| 0                     | 0                            | 160    |
| 1.9                   | 0.81                         | 155    |
| 3.8                   | 27.04                        | 112    |
| 9.4                   | 6.76                         | 96     |
| 14.8                  | 3.24                         | 90     |
| 13.0                  | 4.00                         | 79     |
| 24.1                  | 26.01                        | 56     |
| 24.7                  | $\frac{10.89}{\Sigma=78.75}$ | --**   |

\* by Newton's rule (i.e., trial-and-error procedure) ; (refer to A-23)

$$\begin{aligned}
 f(S) &= a \ln(S/S_0) + b(S - S_0) + t = 0 \\
 &= -2.041 \ln(S/160) + 0.20255(S - 160) + t = 0 \\
 f'(S) &= a/S + b = 0 \\
 &= -2.041/S + 0.20255 = 0
 \end{aligned}$$

for  $t = 0 \rightarrow$  let  $S_i = S_0 = 160$   
 $S_{i+1} = S_i - f(S_i)/f'(S_i)$   
 $= 160 - 0/0.19 = 160$   
 $|S_{i+1} - S_i| = 160 - 160 = 0 < 1E-1$  (convergence value)  
 therefore  $S$  at  $t=0$  is 160 ppm

for  $t=1 \rightarrow$  let  $S_i = 160$   
 $S_{i+1} = S_i - f(S_i)/f'(S_i)$   
 $= 160 - 1/0.19 = 154.7$   
 $|S_{i+1} - S_i| = 160 - 154.7 = 5.3 > 1E-1$   
 let  $S_i = 154.7$   
 $S_{i+1} = 154.7 - (-0.00476)/(0.189) = 154.7$   
 $|S_{i+1} - S_i| = 154.7 - 154.7 = 0 < 1E-1$   
 therefore  $S$  at  $t=1$  is 154.7 ppm

to determine the remaining values of  $S$  at the corresponding values of  $t$ , the basic program on A-24 is used.

\*\*the value of  $Sc$  at  $t = 28$  is indeterminate due to the negative value of  $K$ !

Monod Kinetics (Constant Biomass)

Three-Parameter Model:  $t = \frac{(-K/k)\ln S + (-1/k)S + ((K/k)\ln S_0 + S_0/k)}{y = a x + b z + c}$  ; (refer to A-14)

| <u>y=t</u>  | <u>x=lnS</u>    | <u>z = S</u> | <u>xy</u>       | <u>xz</u>     | <u>yz</u>     | <u>x^2</u>     | <u>z^2</u>     |
|-------------|-----------------|--------------|-----------------|---------------|---------------|----------------|----------------|
| 0           | 5.0752          | 160          | 0               | 812.03        | 0             | 25.76          | 25600          |
| 1           | 5.0106          | 150          | 5.011           | 751.59        | 150           | 25.51          | 22500          |
| 9           | 4.9416          | 140          | 44.474          | 691.82        | 1260          | 24.42          | 19600          |
| 12          | 4.7005          | 110          | 56.406          | 517.05        | 1320          | 22.10          | 12100          |
| 13          | 4.3820          | 80           | 56.966          | 350.56        | 1040          | 19.20          | 6400           |
| 15          | 4.4998          | 90           | 67.497          | 404.98        | 1350          | 20.25          | 8100           |
| 19          | 2.9957          | 20           | 56.918          | 59.91         | 380           | 8.97           | 400            |
| <u>28</u>   | <u>2.3026</u>   | <u>10</u>    | <u>64.473</u>   | <u>23.03</u>  | <u>280</u>    | <u>5.30</u>    | <u>100</u>     |
| $\Sigma=97$ | $\Sigma=33.908$ | $\Sigma=760$ | $\Sigma=351.75$ | $\Sigma=3611$ | $\Sigma=5780$ | $\Sigma=151.1$ | $\Sigma=94800$ |

$A1 = 151.1$  ;  $B1 = 3611$  ;  $C1 = 33.91$  ;  $D1 = 351.75$   
 $A2 = 3611$  ;  $B2 = 94800$  ;  $C2 = 760$  ;  $D2 = 5780$  (refer to A-22)  
 $A3 = 33.91$  ;  $B3 = 760$  ;  $C3 = 8$  ;  $D3 = 97$

$E1 = (3611/151.1) = 23.90$  ;  $F1 = (33.91/151.1) = 0.2244$   
 $E2 = (94800/3611) - 23.90 = 2.355$  ;  $F2 = (760/3611) - 0.2244 = -0.01395$   
 $E3 = (760/33.91) - 23.90 = -1.486$  ;  $F3 = (8/33.91) - 0.2244 = 0.01150$

$G1 = (351.75/151.1) = 2.328$  ;  $H1 = 0.2244 - 23.90 * -0.005924 = 0.3660$   
 $G2 = (5780/3611) - 2.328 = -0.7273$  ;  $H2 = -0.01395/2.355 = -0.005924$   
 $G3 = (97/33.91) - 2.328 = 0.5326$  ;  $H3 = 0.01150/-1.486 - -0.005924 = -0.001815$

$$\begin{aligned}
 I1 &= 2.328 - 23.90 * -0.3088 = 9.709 \\
 I2 &= -0.7273/2.355 = -0.3088 \\
 I3 &= 0.5326/-1.486 - -0.3088 = -0.04958
 \end{aligned}$$

$$\begin{aligned}
 a &= 9.709 - -0.04958 * 0.366 / -0.001815 = -0.2890 \\
 b &= -0.3088 - -0.04958 * -0.005924 / -0.001815 = -0.1470 \\
 c &= -0.04958 / -0.001815 = 27.32
 \end{aligned}$$

$$k = (-1/b) = (-1/-0.1470) = 6.80 \text{ ppm/hr}$$

$$K = (a/b) = (-0.2890/-0.1470) = 1.97 \text{ ppm}$$

| <u>yc = tc = ax + bz + c</u> | <u>(t-tc)^2</u>  | <u>Sc*</u> |
|------------------------------|------------------|------------|
| 2.3                          | 5.29             | 176        |
| 3.8                          | 7.84             | 169        |
| 5.3                          | 13.69            | 115        |
| 9.8                          | 4.84             | 95         |
| 14.3                         | 1.69             | 89         |
| 12.8                         | 4.84             | 75         |
| 23.5                         | 20.25            | 49         |
| 25.2                         | <u>7.84</u>      | .03        |
|                              | $\Sigma = 66.28$ |            |

\*as per Newton's rule (refer to A-20)



Zero-Order Kinetics (Variable Biomass)

One-Parameter Model:  $t = (1/koYc)(\ln(Bo + YcSo - YcS) - \ln(Bo))$ ; (refer to A-7)  
 $y = \quad a \quad \quad \quad x$

| <u>y=t</u> | <u>x=f(S)*</u> | <u>xy</u>          | <u>x^2</u>        | <u>yc=tc=ax</u> | <u>(t-tc)^2</u>  | <u>Sc=f(t)**</u> |
|------------|----------------|--------------------|-------------------|-----------------|------------------|------------------|
| 0          | 0              | 0                  | 0                 | 0               | 0                | 160              |
| 1          | 0.0681         | 0.0681             | 0.00464           | 2.3             | 1.69             | 156              |
| 9          | 0.1318         | 1.1862             | 0.01737           | 4.5             | 20.25            | 117              |
| 12         | 0.3018         | 3.6216             | 0.09108           | 10.3            | 1.70             | 100              |
| 13         | 0.4471         | 5.8123             | 0.19990           | 15.2            | 4.84             | 94               |
| 15         | 0.4010         | 6.0150             | 0.16080           | 13.7            | 1.69             | 81               |
| 19         | 0.6864         | 13.0416            | 0.47114           | 23.4            | 19.36            | 54               |
| 28         | 0.7212         | 20.1936            | 0.52013           | 24.6            | 11.56            | -21              |
|            |                | $\Sigma = 49.9384$ | $\Sigma = 1.4651$ |                 | $\Sigma = 61.09$ |                  |

$$a = \Sigma xy / \Sigma x^2 = (49.9384) / (1.4651) = 34.1 \text{ hr.}$$

$$ko = (1/aYc) = 1/((34.1)(0.136)) = 0.216/\text{hr.}$$

\*  $f(S) = (\ln(Bo + YcSo - YcS) - \ln(Bo))$ , where  $Bo = 19.3$  ppm and  $Yc = 0.136$

\*\*  $f(t) = (Bo + YcSo - Bo \cdot \exp(koYct)) / Yc$

First-Order Kinetics (Variable Biomass)

One-Parameter Model:  $t = (-1/(k_o(Bo+YcSo))) \ln(BoS/((Bo+YcSo-YcS)So))$   
 $y = \quad \quad \quad a \quad \quad \quad x \quad ; \text{ (refer to A-11)}$

| <u>y=t</u> | <u>x=f(S)*</u> | <u>xy</u>          | <u>x^2</u>        | <u>yc=tc=ax</u> | <u>(t-tc)^2</u>   | <u>Sc=f(t)**</u> |
|------------|----------------|--------------------|-------------------|-----------------|-------------------|------------------|
| 0          | 0              | 0                  | 0                 | 0               | 0                 | 160              |
| 1          | -0.1326        | -0.133             | 0.0176            | 1.1             | 0.01              | 151              |
| 9          | -0.2654        | -2.389             | 0.0704            | 2.2             | 46.24             | 84               |
| 12         | -0.6765        | -8.118             | 0.4577            | 5.7             | 39.69             | 64               |
| 13         | -1.1402        | -14.823            | 1.3001            | 9.6             | 11.56             | 58               |
| 15         | -0.9763        | -14.645            | 0.9532            | 8.2             | 46.24             | 48               |
| 19         | -2.7658        | -52.550            | 7.6496            | 23.3            | 18.49             | 32               |
| 28         | -3.4938        | -97.826            | 12.2066           | 29.4            | 1.96              | 12               |
|            |                | $\Sigma = -190.48$ | $\Sigma = 22.655$ |                 | $\Sigma = 164.19$ |                  |

$$a = \Sigma xy / \Sigma x^2 = (-190.48) / (22.655) = -8.408 \text{ hr.}$$

$$k_o = (-1/(a(Bo+YcSo))) = (-1/(-8.408(19.3 + (0.136)(160)))) = 0.00290/\text{ppm hr.}$$

\*  $f(S) = \ln(BoS/((Bo+YcSo-YcS)So))$ , where  $Bo = 19.3$  ppm and  $Yc = 0.136$

\*\*  $Sc = f(t) = (Bo + YcSo)/(Yc + (Bo/So)\exp((Bo+YcSo)kot))$

Monod Kinetics (Variable Biomass)

Two-Parameter Model:  $t = (K/(k_o(Bo+YcSo))) \ln((Bo+YcSo-YcS)So/(BoS))$   
 $+ (1/(k_oYc)) \ln((Bo+YcSo-YcS)/Bo)$

$y = ax+bz$  ; (refer to A-16)

where,

$a = (K/(k_o(Bo+YcSo)))$  ;  $Bo = 19.3$  ppm and  $Yc = 0.136$

$x = \ln((Bo+YcSo-YcS)So/(BoS))$

$b = (1/(k_oYc))$

$z = \ln((Bo+YcSo-YcS)/Bo)$

| <u>y</u> | <u>x</u> | <u>z</u> | <u>xy</u>       | <u>xz</u>        | <u>yz</u>       | <u>x ^ 2</u>    | <u>z ^ 2</u>    |
|----------|----------|----------|-----------------|------------------|-----------------|-----------------|-----------------|
| 0        | 0        | 0        | 0               | 0                | 0               | 0               | 0               |
| 1        | 0.1326   | 0.0681   | 0.1326          | 0.00903          | 0.0681          | 0.01758         | 0.00461         |
| 9        | 0.2654   | 0.1318   | 2.3886          | 0.03498          | 1.1862          | 0.07044         | 0.01737         |
| 12       | 0.6765   | 0.3018   | 8.1180          | 0.20417          | 3.6216          | 0.45765         | 0.09108         |
| 13       | 1.1402   | 0.4471   | 14.8226         | 0.50978          | 5.8123          | 1.30006         | 0.19990         |
| 15       | 0.9763   | 0.4010   | 14.6445         | 0.39150          | 6.0150          | 0.95316         | 0.16080         |
| 19       | 2.7658   | 0.6864   | 52.5502         | 1.89845          | 13.0416         | 7.64965         | 0.47111         |
| 28       | 3.4938   | 0.7212   | 97.8264         | 2.51973          | 20.1936         | 12.20664        | 0.52017         |
|          |          |          | $\Sigma=190.48$ | $\Sigma= 5.5676$ | $\Sigma=49.938$ | $\Sigma=22.655$ | $\Sigma=1.4651$ |

$$a = (\Sigma xy \Sigma z^2 - \Sigma xz \Sigma yz) / (\Sigma x^2 \Sigma z^2 - (\Sigma xz)^2)$$

$$= ((190.48)(1.4651) - (5.5676)(49.938)) / ((22.655)(1.4651) - (5.5676)^2)$$

$$= 0.4729$$

$$b = (\Sigma yz \Sigma x^2 - \Sigma xy \Sigma xz) / (\Sigma x^2 \Sigma z^2 - (\Sigma xz)^2)$$

$$= ((49.938)(22.655) - (190.48)(5.5676)) / ((22.655)(1.4651) - (5.5676)^2)$$

$$= 32.288$$

$$\begin{aligned}
 k_o &= (1/(bY_c)) \\
 &= (1/(32.288*0.136)) \\
 &= 0.228/\text{hr.}
 \end{aligned}$$

$$\begin{aligned}
 K &= (a(B_o+Y_cS_o))/(bY_c) \\
 &= k_o*a(B_o+Y_cS_o) \\
 &= 0.228*0.4729*(19.3+0.136*160) \\
 &= 4.43 \text{ ppm}
 \end{aligned}$$

| <u>yc=tc=ax+bz</u> | <u>(t-tc)^2</u>                  | <u>Sc*</u> |
|--------------------|----------------------------------|------------|
| 0                  | 0                                | 160        |
| 2.3                | 1.69                             | 156        |
| 4.4                | 21.16                            | 116        |
| 10.1               | 3.61                             | 99         |
| 15.0               | 4.00                             | 93         |
| 13.4               | 2.56                             | 80         |
| 23.5               | 20.25                            | 53         |
| 24.9               | 9.61                             | .15        |
|                    | <u><math>\Sigma=62.88</math></u> |            |

\* as per Newton's rule (refer to A-20)

LOTUS 123 SpreadsheetsGeneral Description

Two spreadsheets were created using LOTUS 123 software to facilitate the cumbersome regression calculations demonstrated on the preceding pages of this appendix. The first spreadsheet performs the regression of batch-reactor biodegradation data under the assumption of constant biomass, while the second is for the case in which variable biomass data are available.

The format of the two spreadsheets are identical, as can be seen in the following printouts. The top sheet of each is a summary of inputted data and calculated results. Each subsequent sheet contains the detailed calculations for a given model.

Operation of the spreadsheets involves inputting the following information on the summary sheet: (1) the data reference, (2) the number of data points, and (3) the actual  $S$  vs.  $t$  data. For the case of variable biomass,  $B_0$  and  $Y_c$  must also be inputted. The LOTUS 123 program automatically calculates all the results except for the values of  $Scalc$  for the Monod models. The calculation of  $Scalc$  in the case of the Monod models is accomplished on a Sharp PC-1500 (refer to A-24) using the regressed constants from the spreadsheets. The values of  $Scalc$  must then be inputted on the spreadsheet (i.e., under the "Scalc" column of the Monod sub-sheets) to complete the analysis.

The spreadsheets, as presented, can handle up to 25 ( $S$  vs.  $t$ ) data points. Minor modifications are necessary to increase the capability, if desired.

It should be noted that, although not presented in this appendix, two spreadsheets analogous to those shown here for batch reactor data analysis were developed and used in this thesis for CSTR data analysis. The only notable difference between the two sets of spreadsheets is in the calculation of  $S$  as a function of time (i.e., real time for the batch reactor and residence time for the CSTR). For the case of the CSTR, trial-and-error solution is not required for the Monod equation;  $S$  is directly determined through the use of the quadratic formula for all three of the Monod models, as well as for the first-order variable-biomass model. Caution must be applied when using the quadratic formula in these spreadsheets, however, to ensure that the proper sign (i.e., positive or negative) is used. As a further side note, two variations of the variable-biomass spreadsheet were developed depending on the form of the biomass data (i.e., either  $B_0$  and  $Y_c$  for true CSTR operation or  $B_e$  for the case in which biomass is controlled by recycling/wasting).

---

[illegible]

C-17

Zero-order (1-parameter):  $t = (1/k) * (S_0 - S)$  ; (minimization of  $dt^2$ )

```
----- y=  a  *  x  ; where y=t
```

$$x = (S_0 - S)$$
$$a = (1/k)$$
[illegible]

k = 5.790554 ppm/hr

[illegible]

```
Zero-order (2-parameter):  t=(-1/k)S+(So/k) ; (minimization of dt^2)
-----
y=      a      x+      b      ; where y=t
                                   x=S
                                   a=(-1/k)
                                   b=(So/k)
```

[illegible]
$$k = 6.579330 \text{ ppm/hr}$$

So= 174.7743 ppm



First-order (1-parameter):  $t = (1/k) \ln(S_0/S)$  ; (minimization of  $dt^2$ )

-----  $y = a x$  ; where  $y = t$   
 $x = \ln(S_0/S)$   
 $a = (1/k)$

[illegible]
$$k = 0.092391 \text{ /hr}$$

First-order (2-parameter):  $t = (-1/k) \ln S + (\ln S_0)/k$  ; (minimization of  $dt^2$ )

```
----- y=      a      x +      b      ; where y=t
                                           x=lnS
                                           a=(-1/k)
                                           b=(lnSo)/k
```

[illegible]
$$k = 0.124351 \text{ /hr}$$

So= 313.0210 ppm

$$b = (1/k)$$

[illegible][illegible]

|    |          |     |          |      |          |          |       |          |          |
|----|----------|-----|----------|------|----------|----------|-------|----------|----------|
| 97 | 33.90808 | 760 | 351.7459 | 5780 | 3610.991 | 151.1049 | 94800 | 66.74921 | 2649.656 |
|----|----------|-----|----------|------|----------|----------|-------|----------|----------|

|             |             |             |             |
|-------------|-------------|-------------|-------------|
| A1=151.1049 | B1=3610.991 | C1=33.90808 | D1=351.7459 |
| A2=3610.991 | B2= 94800   | C2= 760     | D2= 5780    |
| A3=33.90808 | B3= 760     | C3= 8       | D3= 97      |

|             |             |             |
|-------------|-------------|-------------|
| E1=23.89724 | F1=0.224400 | G1=2.327825 |
| E2=2.355938 | F2=-0.01393 | G2=-0.72715 |
| E3=-1.48370 | F3=0.011531 | G3=0.532849 |

|             |             |
|-------------|-------------|
| H1=0.365722 | I1=9.703675 |
| H2=-0.00591 | I2=-0.30864 |
| H3=-0.00185 | I3=-0.05048 |

$$k = 6.758245 \text{ ppm/hr}$$

K = 1.576952 ppm

```
a=-0.23333
b=-0.14796
c=27.17090
```

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Variable Biomass

Data source -- Klecka,G.M.,et al (data set #4)

Num.pts.= 8

| Raw    | Data     | Summary of results: |               |          |          |                   |
|--------|----------|---------------------|---------------|----------|----------|-------------------|
| S(ppm) | t(hr)    | Kinetic             | Model         | ko       | K        | avg dt^2 avg dS^2 |
| 160    | 0        | Zero-order          |               |          |          |                   |
| 150    | 1        |                     | (1-parameter) | 0.215716 | ---      | 7.845138 379.4158 |
| 140    | 9        | First-order         |               |          |          |                   |
| 110    | 12       |                     | (1-parameter) | 0.002896 | ---      | 20.42922 946.3390 |
| 80     | 13       | Monod Kinetics      |               |          |          |                   |
| 90     | 15       |                     | (2-parameter) | 0.227597 | 4.375302 | 7.804136 268.9583 |
| 20     | 19       |                     |               |          |          |                   |
| 10     | 28       |                     |               |          |          |                   |
| NA     | NA       |                     |               |          |          |                   |
| NA     | NA       |                     |               |          |          |                   |
| NA     | NA       |                     |               |          |          |                   |
| NA     | NA       |                     |               |          |          |                   |
| NA     | NA       |                     |               |          |          |                   |
| NA     | NA       |                     |               |          |          |                   |
| NA     | NA       |                     |               |          |          |                   |
| NA     | NA       |                     |               |          |          |                   |
| NA     | NA       |                     |               |          |          |                   |
| NA     | NA       |                     |               |          |          |                   |
| NA     | NA       |                     |               |          |          |                   |
| NA     | NA       |                     |               |          |          |                   |
| NA     | NA       |                     |               |          |          |                   |
| NA     | NA       |                     |               |          |          |                   |
| NA     | NA       |                     |               |          |          |                   |
| NA     | NA       |                     |               |          |          |                   |
| NA     | NA       |                     |               |          |          |                   |
| NA     | NA       |                     |               |          |          |                   |
| Bo =   | 19.3 ppm |                     |               |          |          |                   |
| Yc =   | 0.136    |                     |               |          |          |                   |

```
Zero-order (1-parameter): t=(1/koYc)*ln((Bo+YcSo-YcS)/Bo); (min. of dt^2)
----- y=      a      *      x      ;
```

where  $y=t$   
 $x=\ln(B_0+Y_c S_0-Y_c S)/B_0$   
 $a=(1/k_0 Y_c)$

[illegible]

$a = 34.08610$

$$k_o = 0.215716 \text{ /hr}$$

First-order (1-parameter):  $t = -1/(k_o(Bo + Y_c So)) * \ln(BoS / ((Bo + Y_c So - Y_c S) So))$   
 ----- y = a x

```

where y=t
      x=ln(BoS/((Bo+YcSo-YcS)So))
      a=(-1/(ko(Bo+YcSo)))

```

[illegible]
$$a = -8.40782$$
$$k_o = 0.002896 \text{ /ppm-hr}$$

**二、三、四、五、六、七、八、九、十、十一、十二、十三、十四、十五、十六、十七、十八、十九、二十、二十一、二十二、二十三、二十四、二十五、二十六、二十七、二十八、二十九、三十、三十一、三十二、三十三、三十四、三十五、三十六、三十七、三十八、三十九、四十、四十一、四十二、四十三、四十四、四十五、四十六、四十七、四十八、四十九、五十、五十一、五十二、五十三、五十四、五十五、五十六、五十七、五十八、五十九、六十、六十一、六十二、六十三、六十四、六十五、六十六、六十七、六十八、六十九、七十、七十一、七十二、七十三、七十四、七十五、七十六、七十七、七十八、七十九、八十、八十一、八十二、八十三、八十四、八十五、八十六、八十七、八十八、八十九、九十、九十一、九十二、九十三、九十四、九十五、九十六、九十七、九十八、九十九、一百**

where  $y=t$

$$z = \ln((B_0 + Y_c S_0 - Y_c S) / B_0)$$

$$b = (1 / (k_o Y_c))$$

190.4852 49.93938 5.567801 22.65572 1.465095 62.43309 2151.666

$$k_o = 0.227597 \text{ /hr}$$

K = 4.375302 ppm



## Appendix D

### Compilation of Regression Analysis Results for Aerobic Biodegradation Data from Literature Sources

Table of Contents

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| List of Literature References   | D-3            |
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| Index of CSTR Data Analysis Results   | D-8            |
| Regression Analysis Results (for above references,<br>provided in alphabetical order) | D-9 to<br>D-89 |

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Index of Batch Reactor Data Analysis Results

| <u>Reference</u> | <u>Substrate</u>                         | <u>Medium</u>              | <u>Biomass<br/>Type</u> | <u># Sets</u> | <u>Page</u>  |
|------------------|--|----------------------------|-------------------------|---------------|--|
| 1                | 3,4,5-trichloroguaiacol                  | Strain 1395                | Constant                | 3             | D-9 to D-11  |
| 4                | Methylcellulose                          | Activated sludge           | Constant<br>Variable    | 1<br>1        | D-20<br>D-21   |
| 5                | Glucose                                  | Activated sludge           | Constant<br>Variable    | 1<br>1        | D-22<br>D-23   |
| 6                | Peptone/Starch (1:1)                     | Activated sludge           | Constant                | 1             | D-24   |
| 7                | Hexamethylenediamine                     | B.subtilis                 | Constant                | 5             | D-25 to D-29   |
| 8                | Phenol                                   | P.putida                   | Constant<br>Variable    | 1<br>1        | D-30<br>D-31   |
| 9                | $\alpha$ -methylstyrene                  | B.cereus                   | Constant                | 1             | D-34   |
|                  |  | P.aeruginosa               | Constant                | 1             | D-35   |
|                  |  | B.cereus &<br>P.aeruginosa | Constant                | 1             | D-36   |
| 10               | N-nitrosodimethylamine                   | Lake water                 | Constant                | 4             | D-37 to D-40   |
| 11               | Pentachlorophenol                        | Activated sludge           | Constant<br>Variable    | 4<br>4        | D-41, D-43,<br>D-45, D-47<br>D-42, D-44,<br>D-46, D-48 |
| 12               | Octadecyltrimethyl-<br>ammonium chloride | Activated sludge           | Constant                | 1             | D-49   |
| 13               | Fenitrothion                             | Activated sludge           | Constant                | 2             | D-50, D-51   |
|                  | 2,4-dichlorophenoxy-<br>acetic acid      | Activated sludge           | Constant                | 1             | D-52   |
| 14               | Aniline                                  | Pond water                 | Constant                | 2             | D-53, D-54   |
| 15               | 2,4-dichlorophenoxy-<br>acetate          | Activated sludge           | Constant                | 2             | D-55, D-57   |
|                  | Glucose                                  | Activated sludge           | Constant                | 2             | D-56, D-58   |

| <u>Reference</u> | <u>Substrate</u>                 | <u>Medium</u>    | <u>Biomass<br/>Type</u> | <u># Sets</u> | <u>Page</u>        |
|------------------|----------------------------------|------------------|-------------------------|---------------|--------------------|
| 16               | Phenol                           | B.Cereus         | Constant                | 3             | D-59,D-61,<br>D-63 |
|                  |                                  |                  | Variable                | 3             | D-60,D-62,<br>D-64 |
| 17               | Butyl benzyl phthalate           | Activated sludge | Constant                | 1             | D-68               |
|                  | Butylglycolyl butyl<br>phthalate | Activated sludge | Constant                | 1             | D-69               |
| 18               | Phenol                           | Activated sludge | Constant                | 2             | D-70,D-71          |
| 19               | 3,5-dichlorobenzoate             | Activated sludge | Constant                | 1             | D-72               |
|                  |                                  |                  | Variable                | 1             | D-73               |
| 20               | Glucose                          | P.ovalis         | Constant                | 1             | D-74               |
|                  |                                  |                  | Variable                | 1             | D-75               |
| 21               | o-phthalic acid                  | Activated sludge | Constant                | 3             | D-76 to D-78       |
| 22               | 4-chlorobiphenyl                 | Lake water       | Constant                | 1             | D-79               |
|                  | 2-chlorobiphenyl                 | Lake water       | Constant                | 1             | D-80               |
|                  | Biphenyl                         | Lake water       | Constant                | 1             | D-81               |
| 23               | Nitrilotriacetic acid            | Bacterial mutant | Constant                | 1             | D-82               |
|                  |                                  |                  | Variable                | 1             | D-83               |
| 24               | N-nitrosodiethanolamine          | Lake water       | Constant                | 5             | D-84 to D-88       |
|                  |                                  | Activated sludge | Constant                | 1             | D-89               |

Index of CSTR Data Analysis Results

| <u>Reference</u> | <u>Substrate</u>   | <u>Medium</u>    | <u>Biomass<br/>Type</u> | <u># Sets</u> | <u>Page</u>  |
|------------------|--------------------|------------------|-------------------------|---------------|--------------|
| 2                | Phenol             | Activated sludge | Constant                | 2             | D-12, D-14   |
|                  |                    |                  | Variable                | 2             | D-13, D-15   |
| 3                | 2,4-dichlorophenol | Activated sludge | Constant                | 1             | D-16         |
|                  |                    |                  | Variable                | 1             | D-17         |
|                  | Phenol             | Activated sludge | Constant                | 1             | D-18         |
|                  |                    |                  | Variable                | 1             | D-19         |
| 8                | Phenol             | P.putida         | Constant                | 1             | D-32         |
|                  |                    |                  | Variable                | 1             | D-33         |
| 16               | Phenol             | B.cereus         | Constant                | 3             | D-65 to D-67 |



Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Allard,A-C.,et al (data set #1) ; Substrate : 3,4,5-trichloroguaiacol  
Culture : strain 1395

Num.pts.= 14

| Raw Data |       | Summary of results: |          |          |          |          |          |
|----------|-------|---------------------|----------|----------|----------|----------|----------|
| S(ppm)   | t(hr) | Kinetic Model       | k        | K        | So       | avg dt^2 | avg dS^2 |
| 13.8     | 0     | Zero-order          |          |          |          |          |          |
| 13.5     | 12    | (1-parameter)       | 0.018760 | ---      | 13.8     | 429.9616 | 0.151330 |
| 13.7     | 24    | (2-parameter)       | 0.020853 | ---      | 14.19520 | 277.1787 | 0.120535 |
| 13.6     | 36    | First-order         |          |          |          |          |          |
| 13.6     | 48    | (1-parameter)       | 0.001630 | ---      | 13.8     | 669.0595 | 0.222786 |
| 12.5     | 72    | (2-parameter)       | 0.001875 | ---      | 14.46674 | 381.5715 | 0.171876 |
| 12       | 96    | Monod Kinetics      |          |          |          |          |          |
| 12.1     | 120   | (2-parameter)       | 0.007780 | -6.78483 | 13.8     | 304.8192 | 0.112526 |
| 11.5     | 144   | (3-parameter)       | 0.010604 | -5.52034 | 14.0431  | 243.7066 | 0.106820 |
| 10.3     | 168   |                     |          |          |          |          |          |
| 10       | 192   |                     |          |          |          |          |          |
| 10.3     | 216   |                     |          |          |          |          |          |
| 9.5      | 240   |                     |          |          |          |          |          |
| 8.3      | 264   |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Allard,A-C.,et al (data set #2) ; Substrate : 3,4,5-trichloroguaiacol  
Culture : strain 1395

Num.pts.= 13

| Raw Data |       | Summary of results: |          |          |          |          |          |
|----------|-------|---------------------|----------|----------|----------|----------|----------|
| S(ppm)   | t(hr) | Kinetic Model       | k        | K        | So       | avg dt^2 | avg dS^2 |
| 1.31     | 0     | Zero-order          |          |          |          |          |          |
| 1.12     | 12    | (1-parameter)       | 0.006854 | ---      | 1.31     | 1487.169 | 0.069881 |
| 0.95     | 24    | (2-parameter)       | 0.005548 | ---      | 1.099703 | 1210.912 | 0.037285 |
| 0.68     | 48    | First-order         |          |          |          |          |          |
| 0.45     | 72    | (1-parameter)       | 0.016925 | ---      | 1.31     | 153.1641 | 0.002519 |
| 0.33     | 96    | (2-parameter)       | 0.018134 | ---      | 1.645657 | 93.93489 | 0.013272 |
| 0.23     | 120   | Monod Kinetics      |          |          |          |          |          |
| 0.15     | 144   | (2-parameter)       | 0.028253 | 1.298568 | 1.31     | 18.90113 | 0.000630 |
| 0.1      | 168   | (3-parameter)       | 0.024477 | 1.105226 | 1.259    | 16.46033 | 0.000585 |
| 0.06     | 192   |                     |          |          |          |          |          |
| 0.03     | 216   |                     |          |          |          |          |          |
| 0.02     | 240   |                     |          |          |          |          |          |
| 0.01     | 264   |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 92 93 94 95 96 97 98 99 100 101 102 103 104 105 106 107 108 109 110 111 112 113 114 115 116 117 118 119 120 121 122 123 124 125 126 127 128 129 130 131 132 133 134 135 136 137 138 139 140 141 142 143 144 145 146 147 148 149 150 151 152 153 154 155 156 157 158 159 160 161 162 163 164 165 166 167 168 169 170 171 172 173 174 175 176 177 178 179 180 181 182 183 184 185 186 187 188 189 190 191 192 193 194 195 196 197 198 199 200 201 202 203 204 205 206 207 208 209 210 211 212 213 214 215 216 217 218 219 220 221 222 223 224 225 226 227 228 229 230 231 232 233 234 235 236 237 238 239 240 241 242 243 244 245 246 247 248 249 250 251 252 253 254 255 256 257 258 259 260 261 262 263 264 265 266 267 268 269 270 271 272 273 274 275 276 277 278 279 280 281 282 283 284 285 286 287 288 289 290 291 292 293 294 295 296 297 298 299 300 301 302 303 304 305 306 307 308 309 310 311 312 313 314 315 316 317 318 319 320 321 322 323 324 325 326 327 328 329 330 331 332 333 334 335 336 337 338 339 340 341 342 343 344 345 346 347 348 349 350 351 352 353 354 355 356 357 358 359 360 361 362 363 364 365 366 367 368 369 370 371 372 373 374 375 376 377 378 379 380 381 382 383 384 385 386 387 388 389 390 391 392 393 394 395 396 397 398 399 400 401 402 403 404 405 406 407 408 409 410 411 412 413 414 415 416 417 418 419 420 421 422 423 424 425 426 427 428 429 430 431 432 433 434 435 436 437 438 439 440 441 442 443 444 445 446 447 448 449 450 451 452 453 454 455 456 457 458 459 460 461 462 463 464 465 466 467 468 469 470 471 472 473 474 475 476 477 478 479 480 481 482 483 484 485 486 487 488 489 490 491 492 493 494 495 496 497 498 499 500 501 502 503 504 505 506 507 508 509 510 511 512 513 514 515 516 517 518 519 520 521 522 523 524 525 526 527 528 529 530 531 532 533 534 535 536 537 538 539 540 541 542 543 544 545 546 547 548 549 550 551 552 553 554 555 556 557 558 559 560 561 562 563 564 565 566 567 568 569 570 571 572 573 574 575 576 577 578 579 580 581 582 583 584 585 586 587 588 589 590 591 592 593 594 595 596 597 598 599 600 601 602 603 604 605 606 607 608 609 610 611 612 613 614 615 616 617 618 619 620 621 622 623 624 625 626 627 628 629 630 631 632 633 634 635 636 637 638 639 640 641 642 643 644 645 646 647 648 649 650 651 652 653 654 655 656 657 658 659 660 661 662 663 664 665 666 667 668 669 670 671 672 673 674 675 676 677 678 679 680 681 682 683 684 685 686 687 688 689 690 691 692 693 694 695 696 697 698 699 700 701 702 703 704 705 706 707 708 709 710 711 712 713 714 715 716 717 718 719 720 721 722 723 724 725 726 727 728 729 730 731 732 733 734 735 736 737 738 739 740 741 742 743 744 745 746 747 748 749 750 751 752 753 754 755 756 757 758 759 760 761 762 763 764 765 766 767 768 769 770 771 772 773 774 775 776 777 778 779 780 781 782 783 784 785 786 787 788 789 790 791 792 793 794 795 796 797 798 799 800 801 802 803 804 805 806 807 808 809 810 811 812 813 814 815 816 817 818 819 820 821 822 823 824 825 826 827 828 829 830 831 832 833 834 835 836 837 838 839 840 841 842 843 844 845 846 847 848 849 850 851 852 853 854 855 856 857 858 859 860 861 862 863 864 865 866 867 868 869 870 871 872 873 874 875 876 877 878 879 880 881 882 883 884 885 886 887 888 889 890 891 892 893 894 895 896 897 898 899 900 901 902 903 904 905 906 907 908 909 910 911 912 913 914 915 916 917 918 919 920 921 922 923 924 925 926 927 928 929 930 931 932 933 934 935 936 937 938 939 940 941 942 943 944 945 946 947 948 949 950 951 952 953 954 955 956 957 958 959 960 961 962 963 964 965 966 967 968 969 970 971 972 973 974 975 976 977 978 979 980 981 982 983 984 985 986 987 988 989 990 991 992 993 994 995 996 997 998 999 1000 1001 1002 1003 1004 1005 1006 1007 1008 1009 1010 1011 1012 1013 1014 1015 1016 1017 1018 1019 1020 1021 1022 1023 1024 1025 1026 1027 1028 1029 1030 1031 1032 1033 1034 1035 1036 1037 1038 1039 104

Substrate : 3,4,5-trichloroguaiacol  
Culture : strain 1395

Num.pts.= 8

[illegible]

0 100 200 300 400 500 600 700 800 900 1000 1100 1200 1300 1400 1500 1600 1700 1800 1900 2000 2100 2200 2300 2400 2500 2600 2700 2800 2900 3000 3100 3200 3300 3400 3500 3600 3700 3800 3900 4000 4100 4200 4300 4400 4500 4600 4700 4800 4900 5000 5100 5200 5300 5400 5500 5600 5700 5800 5900 6000 6100 6200 6300 6400 6500 6600 6700 6800 6900 7000 7100 7200 7300 7400 7500 7600 7700 7800 7900 8000 8100 8200 8300 8400 8500 8600 8700 8800 8900 9000 9100 9200 9300 9400 9500 9600 9700 9800 9900 10000

[illegible]

lum.ptg.= 7

[illegible]

D-12

REFERS TO RESIDENCE TIME (V/Q)

Regression of CSTR Biodegradation Data (with respect to time) : Variable Biomass Assumed

Data source -- Beltrame,P.,et al,1984 (data set #1) ; Substrate : phenol  
Culture : activated sludge  
Condition : 20C & pH 7.4

Num.pts.= 7

| Raw Data |         |        | Summary of results: |               |          |          |     |          |
|----------|---------|--------|---------------------|---------------|----------|----------|-----|----------|
| Se(ppm)  | Be(ppm) | t(hr)* | Kinetic             | Model         | ko       | K        | Si  | avg dt^2 |
| 180      | 0       | 0      | Zero-order          |               |          |          |     |          |
| 120.6    | 393     | 2.5    |                     | (1-parameter) | 0.044023 | ---      | 180 | 0.379326 |
| 95.1     | 518     | 3      | First-order         |               |          |          |     | 414.2918 |
| 52.7     | 1024    | 3      |                     | (1-parameter) | 0.000794 | ---      | 180 | 0.261224 |
| 52.6     | 1010    | 3      | Monod Kinetics      |               |          |          |     | 87.09340 |
| 41.5     | 968     | 4      |                     | (2-parameter) | 0.093480 | 66.35367 | 180 | 0.000543 |
| 40.1     | 995     | 4      |                     |               |          |          |     | 0.170120 |
| NA       | NA      | NA     |                     |               |          |          |     |          |
| NA       | NA      | NA     |                     |               |          |          |     |          |
| NA       | NA      | NA     |                     |               |          |          |     |          |
| NA       | NA      | NA     |                     |               |          |          |     |          |
| NA       | NA      | NA     |                     |               |          |          |     |          |
| NA       | NA      | NA     |                     |               |          |          |     |          |
| NA       | NA      | NA     |                     |               |          |          |     |          |
| NA       | NA      | NA     |                     |               |          |          |     |          |
| NA       | NA      | NA     |                     |               |          |          |     |          |
| NA       | NA      | NA     |                     |               |          |          |     |          |
| NA       | NA      | NA     |                     |               |          |          |     |          |
| NA       | NA      | NA     |                     |               |          |          |     |          |
| NA       | NA      | NA     |                     |               |          |          |     |          |
| NA       | NA      | NA     |                     |               |          |          |     |          |
| NA       | NA      | NA     |                     |               |          |          |     |          |
| NA       | NA      | NA     |                     |               |          |          |     |          |
| NA       | NA      | NA     |                     |               |          |          |     |          |
| NA       | NA      | NA     |                     |               |          |          |     |          |
| NA       | NA      | NA     |                     |               |          |          |     |          |
| NA       | NA      | NA     |                     |               |          |          |     |          |

\* REFERS TO RESIDENCE TIME (V/Q)

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Num.pts.= 5

D-14

\* REFERS TO RESIDENCE TIME (V/Q)

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Num.pts.= 5

\* REFERS TO RESIDENCE TIME (V/Q)

Culture : mlsa  
Condition : 20C & pH 7.9

9

D-16

\* REFERS TO RESIDENCE TIME (V/Q)



D-17

Regression of CSTR Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Beltrame,P.,et al,1982 (data set #2) ; Substrate : phenol  
Culture : mlss  
Condition : 20C & pH 7.9

Num.pts.= 9

| Raw Data |        | Summary of results: |          |          |          |          |          |
|----------|--------|---------------------|----------|----------|----------|----------|----------|
| Se(ppm)  | t(hr)* | Kinetic Model       | k        | K        | So       | avg dt^2 | avg dS^2 |
| 90       | 0      | Zero-order          |          |          |          |          |          |
| 31       | 6.25   | (1-parameter)       | 4.619440 | ---      | 90       | 48.17293 | 1027.973 |
| 32.8     | 6.25   | (2-parameter)       | 4.641278 | ---      | 90.28087 | 48.17243 | 1037.705 |
| 41.2     | 6.25   | First-order         |          |          |          |          |          |
| 42.9     | 6.25   | (1-parameter)       | 0.195922 | ---      | 90       | 47.50346 | 121.2057 |
| 23.1     | 12.5   | (2-parameter)       | -3.04671 | ---      | -1015.91 | 42.01663 | 136190.3 |
| 26.8     | 12.5   | Monod Kinetics      |          |          |          |          |          |
| 14.9     | 25     | (2-parameter)       | 9.214093 | 25.12215 | 90       | 42.74211 | 228.8289 |
| 45.7     | 25     | (3-parameter)       | 24.13884 | 51.86840 | 134.0115 | 41.77610 | 506.8091 |
| NA       | NA     |                     |          |          |          |          |          |
| NA       | NA     |                     |          |          |          |          |          |
| NA       | NA     |                     |          |          |          |          |          |
| NA       | NA     |                     |          |          |          |          |          |
| NA       | NA     |                     |          |          |          |          |          |
| NA       | NA     |                     |          |          |          |          |          |
| NA       | NA     |                     |          |          |          |          |          |
| NA       | NA     |                     |          |          |          |          |          |
| NA       | NA     |                     |          |          |          |          |          |
| NA       | NA     |                     |          |          |          |          |          |
| NA       | NA     |                     |          |          |          |          |          |
| NA       | NA     |                     |          |          |          |          |          |
| NA       | NA     |                     |          |          |          |          |          |
| NA       | NA     |                     |          |          |          |          |          |
| NA       | NA     |                     |          |          |          |          |          |
| NA       | NA     |                     |          |          |          |          |          |
| NA       | NA     |                     |          |          |          |          |          |

\* REFERS TO RESIDENCE TIME (V/Q)

Regression of CSTR Biodegradation Data (with respect to time) : Variable Biomass Assumed

Data source -- Beltrame,P.,et al,1982 (data set #2) ; Substrate : phenol  
 Culture : activated sludge  
 Condition : 20C & pH 7.9

Num.pts.= 9

| Raw Data |         |        | Summary of results: |          |          |    |                   |
|----------|---------|--------|---------------------|----------|----------|----|-------------------|
| Se(ppm)  | Be(ppm) | t(hr)* | Kinetic Model       | ko       | K        | Si | avg dt^2 avg dS^2 |
| 90       | 0       | 0      | Zero-order          |          |          |    |                   |
| 31       | 299     | 6.25   | (1-parameter)       | 0.031216 | ---      | 90 | 25.81877 952.3909 |
| 32.8     | 257     | 6.25   | First-order         |          |          |    |                   |
| 41.2     | 209     | 6.25   | (1-parameter)       | 0.000933 | ---      | 90 | 1.137048 3.103272 |
| 42.9     | 208     | 6.25   | Monod Kinetics      |          |          |    |                   |
| 23.1     | 237     | 12.5   | (2-parameter)       | 0.200896 | 186.8669 | 90 | 0.430066 2.929465 |
| 26.8     | 185     | 12.5   |                     |          |          |    |                   |
| 14.9     | 208     | 25     |                     |          |          |    |                   |
| 45.7     | 46      | 25     |                     |          |          |    |                   |
| NA       | NA      | NA     |                     |          |          |    |                   |
| NA       | NA      | NA     |                     |          |          |    |                   |
| NA       | NA      | NA     |                     |          |          |    |                   |
| NA       | NA      | NA     |                     |          |          |    |                   |
| NA       | NA      | NA     |                     |          |          |    |                   |
| NA       | NA      | NA     |                     |          |          |    |                   |
| NA       | NA      | NA     |                     |          |          |    |                   |
| NA       | NA      | NA     |                     |          |          |    |                   |
| NA       | NA      | NA     |                     |          |          |    |                   |
| NA       | NA      | NA     |                     |          |          |    |                   |
| NA       | NA      | NA     |                     |          |          |    |                   |
| NA       | NA      | NA     |                     |          |          |    |                   |
| NA       | NA      | NA     |                     |          |          |    |                   |
| NA       | NA      | NA     |                     |          |          |    |                   |
| NA       | NA      | NA     |                     |          |          |    |                   |
| NA       | NA      | NA     |                     |          |          |    |                   |
| NA       | NA      | NA     |                     |          |          |    |                   |

\* REFERS TO RESIDENCE TIME (V/Q)

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Blanchard,F.A.,et al (data set #1) ; Substrate : methylcellulose  
Culture : activated sludge

Num.pts.= 18

| Raw Data |       | Summary of results: |          |          |          |          |          |
|----------|-------|---------------------|----------|----------|----------|----------|----------|
| S(ppm)   | t(hr) | Kinetic Model       | k        | K        | So       | avg dt^2 | avg dS^2 |
| 13.5     | 0     | Zero-order          |          |          |          |          |          |
| 13.2     | 24    | (1-parameter)       | 0.036361 | ---      | 13.5     | 4631.659 | 6.123934 |
| 12.3     | 48    | (2-parameter)       | 0.036718 | ---      | 13.59741 | 4629.990 | 6.242213 |
| 11.1     | 72    | First-order         |          |          |          |          |          |
| 9.9      | 96    | (1-parameter)       | 0.005516 | ---      | 13.5     | 5683.981 | 1.889516 |
| 8.9      | 120   | (2-parameter)       | 0.006411 | ---      | 17.40915 | 5202.202 | 2.213958 |
| 7.3      | 144   | Monod Kinetics      |          |          |          |          |          |
| 4.7      | 168   | (2-parameter)       | 0.034895 | -0.27057 | 13.5     | 4629.916 | ERR      |
| 3.4      | 192   | (3-parameter)       | 0.035577 | -0.18569 | 13.5615  | 4629.414 | ERR      |
| 2.9      | 216   |                     |          |          |          |          |          |
| 2.1      | 240   |                     |          |          |          |          |          |
| 1.8      | 264   |                     |          |          |          |          |          |
| 1.8      | 288   |                     |          |          |          |          |          |
| 2.4      | 312   |                     |          |          |          |          |          |
| 2.6      | 336   |                     |          |          |          |          |          |
| 2.7      | 360   |                     |          |          |          |          |          |
| 3.1      | 408   |                     |          |          |          |          |          |
| 2.7      | 480   |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |

|   |   |   |   |   |   |   |   |   |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |   |
|---|---|---|---|---|---|---|---|---|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|---|
| 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 | 27 | 28 | 29 | 30 | 31 | 32 | 33 | 34 | 35 | 36 | 37 | 38 | 39 | 40 | 41 | 42 | 43 | 44 | 45 | 46 | 47 | 48 | 49 | 50 | 51 | 52 | 53 | 54 | 55 | 56 | 57 | 58 | 59 | 60 | 61 | 62 | 63 | 64 | 65 | 66 | 67 | 68 | 69 | 70 | 71 | 72 | 73 | 74 | 75 | 76 | 77 | 78 | 79 | 80 | 81 | 82 | 83 | 84 | 85 | 86 | 87 | 88 | 89 | 90 | 91 | 92 | 93 | 94 | 95 | 96 | 97 | 98 | 99 | 100 | 101 | 102 | 103 | 104 | 105 | 106 | 107 | 108 | 109 | 110 | 111 | 112 | 113 | 114 | 115 | 116 | 117 | 118 | 119 | 120 | 121 | 122 | 123 | 124 | 125 | 126 | 127 | 128 | 129 | 130 | 131 | 132 | 133 | 134 | 135 | 136 | 137 | 138 | 139 | 140 | 141 | 142 | 143 | 144 | 145 | 146 | 147 | 148 | 149 | 150 | 151 | 152 | 153 | 154 | 155 | 156 | 157 | 158 | 159 | 160 | 161 | 162 | 163 | 164 | 165 | 166 | 167 | 168 | 169 | 170 | 171 | 172 | 173 | 174 | 175 | 176 | 177 | 178 | 179 | 180 | 181 | 182 | 183 | 184 | 185 | 186 | 187 | 188 | 189 | 190 | 191 | 192 | 193 | 194 | 195 | 196 | 197 | 198 | 199 | 200 | 201 | 202 | 203 | 204 | 205 | 206 | 207 | 208 | 209 | 210 | 211 | 212 | 213 | 214 | 215 | 216 | 217 | 218 | 219 | 220 | 221 | 222 | 223 | 224 | 225 | 226 | 227 | 228 | 229 | 230 | 231 | 232 | 233 | 234 | 235 | 236 | 237 | 238 | 239 | 240 | 241 | 242 | 243 | 244 | 245 | 246 | 247 | 248 | 249 | 250 | 251 | 252 | 253 | 254 | 255 | 256 | 257 | 258 | 259 | 260 | 261 | 262 | 263 | 264 | 265 | 266 | 267 | 268 | 269 | 270 | 271 | 272 | 273 | 274 | 275 | 276 | 277 | 278 | 279 | 280 | 281 | 282 | 283 | 284 | 285 | 286 | 287 | 288 | 289 | 290 | 291 | 292 | 293 | 294 | 295 | 296 | 297 | 298 | 299 | 300 | 301 | 302 | 303 | 304 | 305 | 306 | 307 | 308 | 309 | 310 | 311 | 312 | 313 | 314 | 315 | 316 | 317 | 318 | 319 | 320 | 321 | 322 | 323 | 324 | 325 | 326 | 327 | 328 | 329 | 330 | 331 | 332 | 333 | 334 | 335 | 336 | 337 | 338 | 339 | 340 | 341 | 342 | 343 | 344 | 345 | 346 | 347 | 348 | 349 | 350 | 351 | 352 | 353 | 354 | 355 | 356 | 357 | 358 | 359 | 360 | 361 | 362 | 363 | 364 | 365 | 366 | 367 | 368 | 369 | 370 | 371 | 372 | 373 | 374 | 375 | 376 | 377 | 378 | 379 | 380 | 381 | 382 | 383 | 384 | 385 | 386 | 387 | 388 | 389 | 390 | 391 | 392 | 393 | 394 | 395 | 396 | 397 | 398 | 399 | 400 | 401 | 402 | 403 | 404 | 405 | 406 | 407 | 408 | 409 | 410 | 411 | 412 | 413 | 414 | 415 | 416 | 417 | 418 | 419 | 420 | 421 | 422 | 423 | 424 | 425 | 426 | 427 | 428 | 429 | 430 | 431 | 432 | 433 | 434 | 435 | 436 | 437 | 438 | 439 | 440 | 441 | 442 | 443 | 444 | 445 | 446 | 447 | 448 | 449 | 450 | 451 | 452 | 453 | 454 | 455 | 456 | 457 | 458 | 459 | 460 | 461 | 462 | 463 | 464 | 465 | 466 | 467 | 468 | 469 | 470 | 471 | 472 | 473 | 474 | 475 | 476 | 477 | 478 | 479 | 480 | 481 | 482 | 483 | 484 | 485 | 486 | 487 | 488 | 489 | 490 | 491 | 492 | 493 | 494 | 495 | 496 | 497 | 498 | 499 | 500 | 501 | 502 | 503 | 504 | 505 | 506 | 507 | 508 | 509 | 510 | 511 | 512 | 513 | 514 | 515 | 516 | 517 | 518 | 519 | 520 | 521 | 522 | 523 | 524 | 5 |
|---|---|---|---|---|---|---|---|---|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|---|

Num.pts.= 18

D-11

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

data source -- Cech,J.S.,et al (data set #1); Substrate : glucose (measured as COD)  
Culture : activated sludge  
Condition : 20C & pH 7-8

um.pts.= 16

| Raw Data |       | Summary of results: |          |          |          |          |          |  |
|----------|-------|---------------------|----------|----------|----------|----------|----------|--|
| S(ppm)   | t(hr) | Kinetic Model       | k        | K        | So       | avg dt^2 | avg dS^2 |  |
| 970      | 0     | Zero-order          |          |          |          |          |          |  |
| 790      | 0.25  | (1-parameter)       | 195.1849 | ---      | 970      | 0.540649 | 20597.20 |  |
| 702      | 0.5   | (2-parameter)       | 138.0876 | ---      | 791.3305 | 0.243352 | 4640.292 |  |
| 648      | 0.75  | First-order         |          |          |          |          |          |  |
| 584      | 1     | (1-parameter)       | 0.382107 | ---      | 970      | 0.150525 | 2961.212 |  |
| 540      | 1.25  | (2-parameter)       | 0.379627 | ---      | 961.4036 | 0.150336 | 2695.288 |  |
| 520      | 1.5   | Monod Kinetics      |          |          |          |          |          |  |
| 490      | 1.75  | (2-parameter)       | 1086.519 | 2362.418 | 970      | 0.132317 | 4249.814 |  |
| 460      | 2     | (3-parameter)       | 340.3791 | 563.4661 | 841.4649 | 0.087391 | 2205.617 |  |
| 422      | 2.5   |                     |          |          |          |          |          |  |
| 355      | 3     |                     |          |          |          |          |          |  |
| 308      | 3.5   |                     |          |          |          |          |          |  |
| 260      | 4     |                     |          |          |          |          |          |  |
| 205      | 4.5   |                     |          |          |          |          |          |  |
| 160      | 5     |                     |          |          |          |          |          |  |
| 69       | 6     |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Variable Biomass

Data source -- Cech,J.S.,et al (data set #1); Substrate : glucose (measured as COD)  
Culture : activated sludge  
Condition : 20C & pH 7-8

Num.pts.= 16

| Raw Data |         | Summary of results: |          |          |                   |
|----------|---------|---------------------|----------|----------|-------------------|
| S(ppm)   | t(hr)   | Kinetic Model       | ko       | K        | avg dt^2 avg dS^2 |
| 970      | 0       | Zero-order          |          |          |                   |
| 790      | 0.25    | (1-parameter)       | 0.312819 | ---      | 0.971500 101226.8 |
| 702      | 0.5     | First-order         |          |          |                   |
| 648      | 0.75    | (1-parameter)       | 0.000513 | ---      | 0.233862 9499.275 |
| 584      | 1       | Monod Kinetics      |          |          |                   |
| 540      | 1.25    | (2-parameter)       | -0.60848 | -1754.32 | 0.142632 4053.421 |
| 520      | 1.5     |                     |          |          |                   |
| 490      | 1.75    |                     |          |          |                   |
| 460      | 2       |                     |          |          |                   |
| 422      | 2.5     |                     |          |          |                   |
| 355      | 3       |                     |          |          |                   |
| 308      | 3.5     |                     |          |          |                   |
| 260      | 4       |                     |          |          |                   |
| 205      | 4.5     |                     |          |          |                   |
| 160      | 5       |                     |          |          |                   |
| 69       | 6       |                     |          |          |                   |
| NA       | NA      |                     |          |          |                   |
| NA       | NA      |                     |          |          |                   |
| NA       | NA      |                     |          |          |                   |
| NA       | NA      |                     |          |          |                   |
| NA       | NA      |                     |          |          |                   |
| NA       | NA      |                     |          |          |                   |
| NA       | NA      |                     |          |          |                   |
| NA       | NA      |                     |          |          |                   |
| NA       | NA      |                     |          |          |                   |
| Bo =     | 416 ppm |                     |          |          |                   |
| Yc =     | 0.811   |                     |          |          |                   |

|   |   |   |   |   |   |   |   |   |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |   |
|---|---|---|---|---|---|---|---|---|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|---|
| 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 | 27 | 28 | 29 | 30 | 31 | 32 | 33 | 34 | 35 | 36 | 37 | 38 | 39 | 40 | 41 | 42 | 43 | 44 | 45 | 46 | 47 | 48 | 49 | 50 | 51 | 52 | 53 | 54 | 55 | 56 | 57 | 58 | 59 | 60 | 61 | 62 | 63 | 64 | 65 | 66 | 67 | 68 | 69 | 70 | 71 | 72 | 73 | 74 | 75 | 76 | 77 | 78 | 79 | 80 | 81 | 82 | 83 | 84 | 85 | 86 | 87 | 88 | 89 | 90 | 91 | 92 | 93 | 94 | 95 | 96 | 97 | 98 | 99 | 100 | 101 | 102 | 103 | 104 | 105 | 106 | 107 | 108 | 109 | 110 | 111 | 112 | 113 | 114 | 115 | 116 | 117 | 118 | 119 | 120 | 121 | 122 | 123 | 124 | 125 | 126 | 127 | 128 | 129 | 130 | 131 | 132 | 133 | 134 | 135 | 136 | 137 | 138 | 139 | 140 | 141 | 142 | 143 | 144 | 145 | 146 | 147 | 148 | 149 | 150 | 151 | 152 | 153 | 154 | 155 | 156 | 157 | 158 | 159 | 160 | 161 | 162 | 163 | 164 | 165 | 166 | 167 | 168 | 169 | 170 | 171 | 172 | 173 | 174 | 175 | 176 | 177 | 178 | 179 | 180 | 181 | 182 | 183 | 184 | 185 | 186 | 187 | 188 | 189 | 190 | 191 | 192 | 193 | 194 | 195 | 196 | 197 | 198 | 199 | 200 | 201 | 202 | 203 | 204 | 205 | 206 | 207 | 208 | 209 | 210 | 211 | 212 | 213 | 214 | 215 | 216 | 217 | 218 | 219 | 220 | 221 | 222 | 223 | 224 | 225 | 226 | 227 | 228 | 229 | 230 | 231 | 232 | 233 | 234 | 235 | 236 | 237 | 238 | 239 | 240 | 241 | 242 | 243 | 244 | 245 | 246 | 247 | 248 | 249 | 250 | 251 | 252 | 253 | 254 | 255 | 256 | 257 | 258 | 259 | 260 | 261 | 262 | 263 | 264 | 265 | 266 | 267 | 268 | 269 | 270 | 271 | 272 | 273 | 274 | 275 | 276 | 277 | 278 | 279 | 280 | 281 | 282 | 283 | 284 | 285 | 286 | 287 | 288 | 289 | 290 | 291 | 292 | 293 | 294 | 295 | 296 | 297 | 298 | 299 | 300 | 301 | 302 | 303 | 304 | 305 | 306 | 307 | 308 | 309 | 310 | 311 | 312 | 313 | 314 | 315 | 316 | 317 | 318 | 319 | 320 | 321 | 322 | 323 | 324 | 325 | 326 | 327 | 328 | 329 | 330 | 331 | 332 | 333 | 334 | 335 | 336 | 337 | 338 | 339 | 340 | 341 | 342 | 343 | 344 | 345 | 346 | 347 | 348 | 349 | 350 | 351 | 352 | 353 | 354 | 355 | 356 | 357 | 358 | 359 | 360 | 361 | 362 | 363 | 364 | 365 | 366 | 367 | 368 | 369 | 370 | 371 | 372 | 373 | 374 | 375 | 376 | 377 | 378 | 379 | 380 | 381 | 382 | 383 | 384 | 385 | 386 | 387 | 388 | 389 | 390 | 391 | 392 | 393 | 394 | 395 | 396 | 397 | 398 | 399 | 400 | 401 | 402 | 403 | 404 | 405 | 406 | 407 | 408 | 409 | 410 | 411 | 412 | 413 | 414 | 415 | 416 | 417 | 418 | 419 | 420 | 421 | 422 | 423 | 424 | 425 | 426 | 427 | 428 | 429 | 430 | 431 | 432 | 433 | 434 | 435 | 436 | 437 | 438 | 439 | 440 | 441 | 442 | 443 | 444 | 445 | 446 | 447 | 448 | 449 | 450 | 451 | 452 | 453 | 454 | 455 | 456 | 457 | 458 | 459 | 460 | 461 | 462 | 463 | 464 | 465 | 466 | 467 | 468 | 469 | 470 | 471 | 472 | 473 | 474 | 475 | 476 | 477 | 478 | 479 | 480 | 481 | 482 | 483 | 484 | 485 | 486 | 487 | 488 | 489 | 490 | 491 | 492 | 493 | 494 | 495 | 496 | 497 | 498 | 499 | 500 | 501 | 502 | 503 | 504 | 505 | 506 | 507 | 508 | 509 | 510 | 511 | 512 | 513 | 514 | 515 | 516 | 517 | 518 | 519 | 520 | 521 | 522 | 523 | 524 | 5 |
|---|---|---|---|---|---|---|---|---|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|---|

Substrate : peptone/starch @ 1:1 (measured as COD)

Im.pts. = 11

D-24



\_\_\_\_\_

```
data source -- Garbara, S.V., et al (data set #1) ;
```

im.pts.= 8

### Summary of results:

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data source -- Garbara, S.V., et al (data set #2) ;

Substrate : hexamethylenediamine

Culture : Bacillus subtilis (w/montmorillonite)

Condition : 20C & pH 7.3-7.45

um.pts.= 5

Summary of results:

.....

um.pts.= 5

D-27

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num.pts.= 6

Substrate : hexamethylenediamine  
Culture : *Bacillus subtilis* (w/vermiculite)  
Condition : 20C & pH 7.35-7.5

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D-28

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sum.pts.= 5

D-29

D-30

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Variable Biomass

Data source -- Hill,G.A.,et al (data set #1); Substrate : phenol  
Culture : pseudomonas putida  
Condition : 22C & pH 6.2-6.7

Num.pts.= 8

| Raw    | Data  |
|--------|-------|
| S(ppm) | t(hr) |
| 185    | 0     |
| 156    | 11.4  |
| 144    | 13.5  |
| 138    | 14.8  |
| 106    | 15.9  |
| 94     | 16.4  |
| 59     | 17.3  |
| 31     | 17.9  |
| NA     | NA    |
| NA     | NA    |
| NA     | NA    |
| NA     | NA    |
| NA     | NA    |
| NA     | NA    |
| NA     | NA    |
| NA     | NA    |
| NA     | NA    |
| NA     | NA    |
| NA     | NA    |
| NA     | NA    |
| NA     | NA    |
| NA     | NA    |
| NA     | NA    |

Summary of results:

| Kinetic        | Model         | ka       | K        | avg dt^2 | avg dS^2 |
|----------------|---------------|----------|----------|----------|----------|
| Zero-order     |               |          |          |          |          |
|                | (1-parameter) | 0.170988 | ---      | 6.240491 | 565.7221 |
| First-order    |               |          |          |          |          |
|                | (1-parameter) | 0.001352 | ---      | 20.31234 | 1004.337 |
| Monod Kinetics |               |          |          |          |          |
|                | (2-parameter) | 0.086218 | -65.7635 | 1.506825 | 796.8413 |

Bo = 14.3 ppm  
Yc = 0.52

.....

[illegible]

n.pts.= 7

[illegible]

REFERS TO RESIDENCE TIME (V/Q)



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[illegible]

pts.= 7

[illegible]

REFERS TO RESIDENCE TIME (V/Q)

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Num.pts.= 6

D-34

1000 1001 1002 1003 1004 1005 1006 1007 1008 1009 1010 1011 1012 1013 1014 1015 1016 1017 1018 1019 1020 1021 1022 1023 1024 1025 1026 1027 1028 1029 1030 1031 1032 1033 1034 1035 1036 1037 1038 1039 1040 1041 1042 1043 1044 1045 1046 1047 1048 1049 1050 1051 1052 1053 1054 1055 1056 1057 1058 1059 1060 1061 1062 1063 1064 1065 1066 1067 1068 1069 1070 1071 1072 1073 1074 1075 1076 1077 1078 1079 1080 1081 1082 1083 1084 1085 1086 1087 1088 1089 1090 1091 1092 1093 1094 1095 1096 1097 1098 1099 1100 1101 1102 1103 1104 1105 1106 1107 1108 1109 1110 1111 1112 1113 1114 1115 1116 1117 1118 1119 1120 1121 1122 1123 1124 1125 1126 1127 1128 1129 1130 1131 1132 1133 1134 1135 1136 1137 1138 1139 1140 1141 1142 1143 1144 1145 1146 1147 1148 1149 1150 1151 1152 1153 1154 1155 1156 1157 1158 1159 1160 1161 1162 1163 1164 1165 1166 1167 1168 1169 1170 1171 1172 1173 1174 1175 1176 1177 1178 1179 1180 1181 1182 1183 1184 1185 1186 1187 1188 1189 1190 1191 1192 1193 1194 1195 1196 1197 1198 1199 1200 1201 1202 1203 1204 1205 1206 1207 1208 1209 1210 1211 1212 1213 1214 1215 1216 1217 1218 1219 1220 1221 1222 1223 1224 1225 1226 1227 1228 1229 1230 1231 1232 1233 1234 1235 1236 1237 1238 1239 1240 1241 1242 1243 1244 1245 1246 1247 1248 1249 1250 1251 1252 1253 1254 1255 1256 1257 1258 1259 1260 1261 1262 1263 1264 1265 1266 1267 1268 1269 1270 1271 1272 1273 1274 1275 1276 1277 1278 1279 1280 1281 1282 1283 1284 1285 1286 1287 1288 1289 1290 1291 1292 1293 1294 1295 1296 1297 1298 1299 1300 1301 1302 1303 1304 1305 1306 1307 1308 1309 1310 1311 1312 1313 1314 1315 1316 1317 1318 1319 1320 1321 1322 1323 1324 1325 1326 1327 1328 1329 1330 1331 1332 1333 1334 1335 1336 1337 1338 1339 1340 1341 1342 1343 1344 1345 1346 1347 1348 1349 1350 1351 1352 1353 1354 1355 1356 1357 1358 1359 1360 1361 1362 1363 1364 1365 1366 1367 1368 1369 1370 1371 1372 1373 1374 1375 1376 1377 1378 1379 1380 1381 1382 1383 1384 1385 1386 1387 1388 1389 1390 1391 1392 1393 1394 1395 1396 1397 1398 1399 1400 1401 1402 1403 1404 1405 1406 1407 1408 1409 1410 1411 1412 1413 1414 1415 1416 1417 1418 1419 1420 1421 1422 1423 1424 1425 1426 1427 1428 1429 1430 1431 1432 1433 1434 1435 1436 1437 1438 1439 1440 1441 1442 1443 1444 1445 1446 1447 1448 1449 1450 1451 1452 1453 1454 1455 1456 1457 1458 1459 1460 1461 1462 1463 1464 1465 1466 1467 1468 1469 1470 1471 1472 1473 1474 1475 1476 1477 1478 1479 1480 1481 1482 1483 1484 1485 1486 1487 1488 1489 1490 1491 1492 1493 1494 1495 1496 1497 1498 1499 1500 1501 1502 1503 1504 1505 1506 1507 1508 1509 1510 1511 1512 1513 1514 1515 1516 1517 1518 1519 1520 1521 1522 1523 1524 1525 1526 1527 1528 1529 1530 1531 1532 1533 1534 1535 1536 1537 1538 1539 1540 1541 1542 1543 1544 1545 1546 1547 1548 1549 1550 1551 1552 1553 1554 1555 1556 1557 1558 1559 1560 1561 1562 1563 1564 1565 1566 1567 1568 1569 1570 1571 1572 1573 1574 1575 1576 1577 1578 1579 1580 1581 1582 1583 1584 1585 1586 1587 1588 1589 1590 1591 1592 1593 1594 1595 1596 1597 1598 1599 1600 1601 1602 1603 1604 1605 1606 1607 1608 1609 1610 1611 1612 1613 1614 1615 1616 1617 1618 1619 1620 1621 1622 1623 1624 1625 1626 1627 1628 1629 1630 1631 1632 1633 1634 1635 1636 1637 1638 1639 1640 1641 1642 1643 1644 1645 1646 1647 1648 1649 1650 1651 1652 1653 1654 1655 1656 1657 1658 1659 1660 1661 1662 1663 1664 1665 1666 1667 1668 1669 1670 1671 1672 1673 1674 1675 1676 1677 1678 1679 1680 1681 1682 1683 1684 1685 1686 1687 1688 1689 1690 1691 1692 1693 1694 1695 1696 1697 1698 1699 1700 1701 1702 1703 1704 1705 1706 1707 1708 1709 1710 1711 1712 1713 1714 1715 1716 1717 1718 1719 1720 1721 1722 1723 1724 1725 1726 1727 1728 1729 1730 1731 1732 1733 1734 1735 1736 1737 1738 1739 1740 1741 1742 1743 1744 1745 1746 1747 1748 1749 1750 1751 1752 1753 1754 1755 1756 1757 1758 1759 1760 1761 1762 1763 1764 1765 1766 1767 1768 1769 1770 1771 1772 1773 1774 1775 1776 1777 1778 1779 1780 1781 1782 1783 1784 1785 1786 1787 1788 1789 1790 1791 1792 1793 1794 1795 1796 1797 1798 1799 1800 1801 1802 1803 1804 1805 1806 1807 1808 1809 1810 1811 1812 1813 1814 1815 1816 1817 1818

Num.pts.= 6

[illegible]

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Num.pts.= 4

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Substrate : N-nitrosodimethylamine  
Culture : Lake Cochituate water  
Condition : room temperature & pH 6-7

Num.pts.= 13

[illegible]

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Kaplan,D.L. and Kaplan A.M. (data set #2) ; Substrate : N-nitrosodimethylamine  
 Culture : Lake Cochituate water  
 Condition : room temperature & pH 6-7

Num.pts.= 13

| Raw Data |       | Summary of results: |           |          |          |          |          |
|----------|-------|---------------------|-----------|----------|----------|----------|----------|
| S(ppm)   | t(hr) | Kinetic Model       | k         | K        | So       | avg dt^2 | avg dS^2 |
| 1.5      | 0     | Zero-order          |           |          |          |          |          |
| 1.57     | 86    | (1-parameter)       | 0.000441  | ---      | 1.5      | 78959.97 | 0.015394 |
| 1.51     | 144   | (2-parameter)       | 0.000301  | ---      | 1.408627 | 67837.68 | 0.006183 |
| 1.28     | 192   | First-order         |           |          |          |          |          |
| 1.25     | 276   | (1-parameter)       | 0.000326  | ---      | 1.5      | 74694.94 | 0.011263 |
| 1.22     | 360   | (2-parameter)       | 0.000225  | ---      | 1.403080 | 63472.53 | 0.004700 |
| 1.2      | 456   | Monod Kinetics      |           |          |          |          |          |
| 1.19     | 540   | (2-parameter)       | -0.000002 | -1.41085 | 1.5      | 32425.17 | 0.000818 |
| 1.18     | 708   | (3-parameter)       | -0.000001 | -1.39829 | 1.473    | 31904.24 | 0.000861 |
| 1.18     | 792   |                     |           |          |          |          |          |
| 1.18     | 948   |                     |           |          |          |          |          |
| 1.17     | 1116  |                     |           |          |          |          |          |
| 1.17     | 1368  |                     |           |          |          |          |          |
| NA       | NA    |                     |           |          |          |          |          |
| NA       | NA    |                     |           |          |          |          |          |
| NA       | NA    |                     |           |          |          |          |          |
| NA       | NA    |                     |           |          |          |          |          |
| NA       | NA    |                     |           |          |          |          |          |
| NA       | NA    |                     |           |          |          |          |          |
| NA       | NA    |                     |           |          |          |          |          |
| NA       | NA    |                     |           |          |          |          |          |
| NA       | NA    |                     |           |          |          |          |          |
| NA       | NA    |                     |           |          |          |          |          |
| NA       | NA    |                     |           |          |          |          |          |
| NA       | NA    |                     |           |          |          |          |          |
| NA       | NA    |                     |           |          |          |          |          |
| NA       | NA    |                     |           |          |          |          |          |

# Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Kaplan,D.L. and Kaplan A.M. (data set #3) ; Substrate : N-nitrosodimethylamine  
 Culture : Lake Cochituate water  
 Condition : room temperature & pH 6-7

Num.pts.= 13

| Raw Data |       | Summary of results: |  |           |          |          |                     |                     |
|----------|-------|---------------------|--|-----------|----------|----------|---------------------|---------------------|
| S(ppm)   | t(hr) | Kinetic Model       |  | k         | K        | So       | avg dt <sup>2</sup> | avg dS <sup>2</sup> |
| 0.15     | 0     | Zero-order          |  |           |          |          |                     |                     |
| 0.126    | 96    | (1-parameter)       |  | 0.000058  | ---      | 0.15     | 57869.93            | 0.000200            |
| 0.131    | 144   | (2-parameter)       |  | 0.000043  | ---      | 0.139461 | 48439.72            | 0.000092            |
| 0.128    | 192   | First-order         |  |           |          |          |                     |                     |
| 0.119    | 276   | (1-parameter)       |  | 0.000459  | ---      | 0.15     | 51361.43            | 0.000123            |
| 0.111    | 360   | (2-parameter)       |  | 0.000350  | ---      | 0.138961 | 42950.83            | 0.000061            |
| 0.109    | 456   | Monod Kinetics      |  |           |          |          |                     |                     |
| 0.107    | 540   | (2-parameter)       |  | -0.000000 | -0.14116 | 0.15     | 29192.39            | 0.000022            |
| 0.105    | 708   | (3-parameter)       |  | -0.000000 | -0.13657 | ERR      | 21725.37            | ERR                 |
| 0.104    | 792   |                     |  |           |          |          |                     |                     |
| 0.104    | 948   |                     |  |           |          |          |                     |                     |
| 0.103    | 1116  |                     |  |           |          |          |                     |                     |
| 0.101    | 1368  |                     |  |           |          |          |                     |                     |
| NA       | NA    |                     |  |           |          |          |                     |                     |
| NA       | NA    |                     |  |           |          |          |                     |                     |
| NA       | NA    |                     |  |           |          |          |                     |                     |
| NA       | NA    |                     |  |           |          |          |                     |                     |
| NA       | NA    |                     |  |           |          |          |                     |                     |
| NA       | NA    |                     |  |           |          |          |                     |                     |
| NA       | NA    |                     |  |           |          |          |                     |                     |
| NA       | NA    |                     |  |           |          |          |                     |                     |
| NA       | NA    |                     |  |           |          |          |                     |                     |
| NA       | NA    |                     |  |           |          |          |                     |                     |
| NA       | NA    |                     |  |           |          |          |                     |                     |
| NA       | NA    |                     |  |           |          |          |                     |                     |

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Kaplan,D.L. and Kaplan A.M. (data set #4) ; Substrate : N-nitrosodimethylamine  
 Culture : Lake Cochituate water  
 Condition : room temperature & pH 6-7

Num.pts.= 13

| Raw Data |       |
|----------|-------|
| S(ppm)   | t(hr) |
| 0.015    | 0     |
| 0.0134   | 96    |
| 0.0129   | 144   |
| 0.0122   | 192   |
| 0.0111   | 276   |
| 0.0087   | 360   |
| 0.0069   | 456   |
| 0.0059   | 540   |
| 0.0056   | 708   |
| 0.0053   | 792   |
| 0.0051   | 948   |
| 0.005    | 1116  |
| 0.0049   | 1368  |
| NA       | NA    |
| NA       | NA    |
| NA       | NA    |
| NA       | NA    |
| NA       | NA    |
| NA       | NA    |
| NA       | NA    |
| NA       | NA    |
| NA       | NA    |
| NA       | NA    |
| NA       | NA    |

Summary of results:

| Kinetic Model  | k        | K        | So       | avg dt^2 | avg dS^2 |
|----------------|----------|----------|----------|----------|----------|
| Zero-order     |          |          |          |          |          |
| (1-parameter)  | 0.000011 | ---      | 0.015    | 37856.23 | 4.89E-06 |
| (2-parameter)  | 0.000010 | ---      | 0.014025 | 35565.54 | 3.59E-06 |
| First-order    |          |          |          |          |          |
| (1-parameter)  | 0.001169 | ---      | 0.015    | 26953.21 | 1.16E-06 |
| (2-parameter)  | 0.001117 | ---      | 0.014399 | 26557.87 | 1.12E-06 |
| Monod Kinetics |          |          |          |          |          |
| (2-parameter)  | -8.5E-06 | -0.01686 | 0.015    | 21741.60 | 1.30E-06 |
| (3-parameter)  | -4.9E-06 | -0.01303 | ERR      | 19323.44 | ERR      |



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Substrate : pentachlorophenol

**Appendix A**

Condition : 22C & neutral pH

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\*\*K has units of ppb.

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Condition : 22C & neutral pH

Num.pts.= 8

[illegible]

Bo = 20.8 ppb  
Yc = 0.136

\*k<sub>0</sub> has units of ppb/ppb-hr for zero-order/Monod & 1/ppb-hr for 1st-order kinetics.  
 \*\*K has units of ppb.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Klecka,G.M.,et al (data set #2) ; Substrate : pentachlorophenol  
 Culture : mlss  
 Condition : 22C & neutral pH

Num.pts.= 9

| Raw Data |       | Summary of results: |          |          |          |          |          |
|----------|-------|---------------------|----------|----------|----------|----------|----------|
| s(ppb)   | t(hr) | Kinetic Model       | k *      | K **     | So       | avg dt^2 | avg dS^2 |
| 800      | 0     | Zero-order          |          |          |          |          |          |
| 770      | 2     | (1-parameter)       | 13.77015 | ---      | 800      | 53.36714 | 10119.32 |
| 790      | 9     | (2-parameter)       | 17.24581 | ---      | 925.8672 | 20.63294 | 6136.612 |
| 730      | 13    | First-order         |          |          |          |          |          |
| 710      | 15    | (1-parameter)       | 0.077573 | ---      | 800      | 192.7163 | 127735.4 |
| 700      | 19    | (2-parameter)       | 0.108348 | ---      | 3091.231 | 66.61709 | 965473.0 |
| 550      | 27    | Monod Kinetics      |          |          |          |          |          |
| 410      | 31    | (2-parameter)       | 8.897153 | -79.3392 | 800      | 29.79181 | 10523.60 |
| 10       | 50    | (3-parameter)       | 11.99347 | -59.1626 | 872.473  | 15.17606 | 5790.434 |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |

\* k has units of ppb/hr for zero-order/Monod kinetics.  
 \*\*K has units of ppb.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Variable Biomass

Data source -- Klecka,G.M.,et al (data set #2) ; Substrate : pentachlorophenol  
Culture : mlss  
Condition : 22C & neutral pH

Num.pts.= 9

| Raw Data |        | Summary of results: |          |          |                   |
|----------|--------|---------------------|----------|----------|-------------------|
| s (ppb)  | t (hr) | Kinetic Model       | ko*      | K**      | avg dt^2 avg dS^2 |
| 800      | 0      | Zero-order          |          |          |                   |
| 770      | 2      | (1-parameter)       | 0.369319 | ---      | 10.78251 2925.519 |
| 790      | 9      | First-order         |          |          |                   |
| 730      | 13     | (1-parameter)       | 0.000945 | ---      | 65.30591 23907.72 |
| 710      | 15     | Monod Kinetics      |          |          |                   |
| 700      | 19     | (2-parameter)       | 0.420010 | 60.59482 | 9.573569 830.2494 |
| 550      | 27     |                     |          |          |                   |
| 410      | 31     |                     |          |          |                   |
| 10       | 50     |                     |          |          |                   |
| NA       | NA     |                     |          |          |                   |
| NA       | NA     |                     |          |          |                   |
| NA       | NA     |                     |          |          |                   |
| NA       | NA     |                     |          |          |                   |
| NA       | NA     |                     |          |          |                   |
| NA       | NA     |                     |          |          |                   |
| NA       | NA     |                     |          |          |                   |
| NA       | NA     |                     |          |          |                   |
| NA       | NA     |                     |          |          |                   |
| NA       | NA     |                     |          |          |                   |
| NA       | NA     |                     |          |          |                   |
| NA       | NA     |                     |          |          |                   |
| NA       | NA     |                     |          |          |                   |
| NA       | NA     |                     |          |          |                   |
| NA       | NA     |                     |          |          |                   |
| NA       | NA     |                     |          |          |                   |

Bo = 11 ppb  
Yc = 0.136

\* ko has units of ppb/ppb-hr for zero-order/Monod & 1/ppb-hr for 1st-order kinetics.  
\*\*K has units of ppb.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Klecka,G.M.,et al (data set #3) ; Substrate : pentachlorophenol  
Culture : mlss  
Condition : 22C & neutral pH

Num.pts.= 9

| Raw Data |       | Summary of results: |          |          |          |          |          |  |
|----------|-------|---------------------|----------|----------|----------|----------|----------|--|
| S (ppb)  | t(hr) | Kinetic Model       | k *      | K**      | So       | avg dt^2 | avg dS^2 |  |
| 410      | 0     | Zero-order          |          |          |          |          |          |  |
| 390      | 2     | (1-parameter)       | 11.34194 | ---      | 410      | 4.160506 | 535.2061 |  |
| 330      | 8     | (2-parameter)       | 12.29912 | ---      | 432.4308 | 2.947864 | 445.9191 |  |
| 300      | 13    | First-order         |          |          |          |          |          |  |
| 260      | 14    | (1-parameter)       | 0.085683 | ---      | 410      | 81.02445 | 10953.29 |  |
| 220      | 19    | (2-parameter)       | 0.127002 | ---      | 1231.004 | 34.88447 | 115547.5 |  |
| 170      | 24    | Monod Kinetics      |          |          |          |          |          |  |
| 80       | 28    | (2-parameter)       | 9.387858 | -28.1195 | 410      | 1.357258 | 373.0343 |  |
| 10       | 32    | (3-parameter)       | 9.810835 | -26.0584 | 417.032  | 1.230424 | 310.6863 |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |

\* k has units of ppb/hr for zero-order/Monod kinetics.  
\*\*K has units of ppb.

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Condition : 22C & neutral pH

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| Kinetic Model  | $k_o^*$  | $K^{**}$ | avg dt <sup>2</sup> | avg dS <sup>2</sup> |
|----------------|----------|----------|---------------------|---------------------|
| Zero-order     |          |          |                     |                     |
| (1-parameter)  | 0.324746 | ---      | 1.875002            | 348.4533            |
| First-order    |          |          |                     |                     |
| (1-parameter)  | 0.001620 | ---      | 32.12857            | 3728.398            |
| Monod Kinetics |          |          |                     |                     |
| (2-parameter)  | 0.364380 | 27.12973 | 1.359894            | 229.7172            |

Bo = 18.9 ppb  
Yc = 0.136

\* ko has units of ppb/ppb-hr for zero-order/Monod & 1/ppb/hr for 1st-order kinetics.  
\*\*K has units of ppb.

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 92 93 94 95 96 97 98 99 100 101 102 103 104 105 106 107 108 109 110 111 112 113 114 115 116 117 118 119 120 121 122 123 124 125 126 127 128 129 130 131 132 133 134 135 136 137 138 139 140 141 142 143 144 145 146 147 148 149 150 151 152 153 154 155 156 157 158 159 160 161 162 163 164 165 166 167 168 169 170 171 172 173 174 175 176 177 178 179 180 181 182 183 184 185 186 187 188 189 190 191 192 193 194 195 196 197 198 199 200 201 202 203 204 205 206 207 208 209 210 211 212 213 214 215 216 217 218 219 220 221 222 223 224 225 226 227 228 229 230 231 232 233 234 235 236 237 238 239 240 241 242 243 244 245 246 247 248 249 250 251 252 253 254 255 256 257 258 259 260 261 262 263 264 265 266 267 268 269 270 271 272 273 274 275 276 277 278 279 280 281 282 283 284 285 286 287 288 289 290 291 292 293 294 295 296 297 298 299 300 301 302 303 304 305 306 307 308 309 310 311 312 313 314 315 316 317 318 319 320 321 322 323 324 325 326 327 328 329 330 331 332 333 334 335 336 337 338 339 340 341 342 343 344 345 346 347 348 349 350 351 352 353 354 355 356 357 358 359 360 361 362 363 364 365 366 367 368 369 370 371 372 373 374 375 376 377 378 379 380 381 382 383 384 385 386 387 388 389 390 391 392 393 394 395 396 397 398 399 400 401 402 403 404 405 406 407 408 409 410 411 412 413 414 415 416 417 418 419 420 421 422 423 424 425 426 427 428 429 430 431 432 433 434 435 436 437 438 439 440 441 442 443 444 445 446 447 448 449 450 451 452 453 454 455 456 457 458 459 460 461 462 463 464 465 466 467 468 469 470 471 472 473 474 475 476 477 478 479 480 481 482 483 484 485 486 487 488 489 490 491 492 493 494 495 496 497 498 499 500 501 502 503 504 505 506 507 508 509 510 511 512 513 514 515 516 517 518 519 520 521 522 523 524 525 526 527 528 529 530 531 532 533 534 535 536 537 538 539 540 541 542 543 544 545 546 547 548 549 550 551 552 553 554 555 556 557 558 559 560 561 562 563 564 565 566 567 568 569 570 571 572 573 574 575 576 577 578 579 580 581 582 583 584 585 586 587 588 589 590 591 592 593 594 595 596 597 598 599 600 601 602 603 604 605 606 607 608 609 610 611 612 613 614 615 616 617 618 619 620 621 622 623 624 625 626 627 628 629 630 631 632 633 634 635 636 637 638 639 640 641 642 643 644 645 646 647 648 649 650 651 652 653 654 655 656 657 658 659 660 661 662 663 664 665 666 667 668 669 670 671 672 673 674 675 676 677 678 679 680 681 682 683 684 685 686 687 688 689 690 691 692 693 694 695 696 697 698 699 700 701 702 703 704 705 706 707 708 709 710 711 712 713 714 715 716 717 718 719 720 721 722 723 724 725 726 727 728 729 730 731 732 733 734 735 736 737 738 739 740 741 742 743 744 745 746 747 748 749 750 751 752 753 754 755 756 757 758 759 760 761 762 763 764 765 766 767 768 769 770 771 772 773 774 775 776 777 778 779 780 781 782 783 784 785 786 787 788 789 790 791 792 793 794 795 796 797 798 799 800 801 802 803 804 805 806 807 808 809 810 811 812 813 814 815 816 817 818 819 820 821 822 823 824 825 826 827 828 829 830 831 832 833 834 835 836 837 838 839 840 841 842 843 844 845 846 847 848 849 850 851 852 853 854 855 856 857 858 859 860 861 862 863 864 865 866 867 868 869 870 871 872 873 874 875 876 877 878 879 880 881 882 883 884 885 886 887 888 889 890 891 892 893 894 895 896 897 898 899 900 901 902 903 904 905 906 907 908 909 910 911 912 913 914 915 916 917 918 919 920 921 922 923 924 925 926 927 928 929 930 931 932 933 934 935 936 937 938 939 940 941 942 943 944 945 946 947 948 949 950 951 952 953 954 955 956 957 958 959 960 961 962 963 964 965 966 967 968 969 970 971 972 973 974 975 976 977 978 979 980 981 982 983 984 985 986 987 988 989 990 991 992 993 994 995 996 997 998 999 1000 1001 1002 1003 1004 1005 1006 1007 1008 1009 1010 1011 1012 1013 1014 1015 1016 1017 1018 1019 1020 1021 1022 1023 1024 1025 1026 1027 1028 1029 1030 1031 1032 1033 1034 1035 1036 1037 1038 1039 1040 1

Substrate : pentachlorophenol  
Culture : m1ss  
Condition : 22C & neutral pH

Condition : 22C & neutral pH

D-47

```
* k has units of ppb/hr for zero-order/Monod kinetics.
**K has units of ppb.
```

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Variable Biomass

Data source -- Klecka,G.M.,et al (data set #4) ; Substrate : pentachlorophenol  
 Culture : mlss  
 Condition : 22C & neutral pH

Num.pts.= 8

| Raw Data | Summary of results: |                |          |          |                   |
|----------|---------------------|----------------|----------|----------|-------------------|
| S (ppb)  | t(hr)               | Kinetic Model  | ko*      | K**      | avg dt^2 avg dS^2 |
| 160      | 0                   | Zero-order     |          |          |                   |
| 150      | 1                   | (1-parameter)  | 0.215716 | ---      | 7.845138 379.4158 |
| 140      | 9                   | First-order    |          |          |                   |
| 110      | 12                  | (1-parameter)  | 0.002896 | ---      | 20.42922 946.3390 |
| 80       | 13                  | Monod Kinetics |          |          |                   |
| 90       | 15                  | (2-parameter)  | 0.227597 | 4.375302 | 7.804136 268.9583 |
| 20       | 19                  |                |          |          |                   |
| 10       | 28                  |                |          |          |                   |
| NA       | NA                  |                |          |          |                   |
| NA       | NA                  |                |          |          |                   |
| NA       | NA                  |                |          |          |                   |
| NA       | NA                  |                |          |          |                   |
| NA       | NA                  |                |          |          |                   |
| NA       | NA                  |                |          |          |                   |
| NA       | NA                  |                |          |          |                   |
| NA       | NA                  |                |          |          |                   |
| NA       | NA                  |                |          |          |                   |
| NA       | NA                  |                |          |          |                   |
| NA       | NA                  |                |          |          |                   |
| NA       | NA                  |                |          |          |                   |
| NA       | NA                  |                |          |          |                   |
| NA       | NA                  |                |          |          |                   |
| NA       | NA                  |                |          |          |                   |
| NA       | NA                  |                |          |          |                   |
| NA       | NA                  |                |          |          |                   |
| NA       | NA                  |                |          |          |                   |
| NA       | NA                  |                |          |          |                   |

Bo = 19.3 ppb  
 Yc = 0.136

\* ko has units of ppb/ppb-hr for zero-order/Monod & 1/ppb-hr for 1st-order kinetics.  
 \*\*K has units of ppb.



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Num.pts.= 6

D-49

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[illegible]

Sum.pts.= 7

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Num.pts.= 7

D-51

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Data source -- Liu,D.,et al (data set #3) ; Substrate : 2,4-dichlorophenoxyacetic acid  
Culture : activated sludge  
Condition : 22C & pH 6.8

Num.pts.= 6

.....

Substrate : aniline

Condition : room temperature/neutral pH

Condition : room temperature/neutral pH

D-53

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Substrate : aniline

Condition : room temperature/neutral pH

Condition : room temperature/neutral pH

8

1990 1991 1992 1993 1994 1995 1996 1997 1998 1999 2000 2001 2002 2003 2004 2005 2006 2007 2008 2009

| Kinetic Model  | k        | K        | So       | avg dt <sup>2</sup> | avg dS <sup>2</sup> |
|----------------|----------|----------|----------|---------------------|---------------------|
| Zero-order     |          |          |          |                     |                     |
| (1-parameter)  | 2.205679 | ---      | 250      | 1304.471            | 6346.280            |
| (2-parameter)  | 1.796770 | ---      | 208.8037 | 1233.287            | 3981.525            |
| First-order    |          |          |          |                     |                     |
| (1-parameter)  | 0.023695 | ---      | 250      | 331.0626            | 628.9022            |
| (2-parameter)  | 0.019883 | ---      | 164.0943 | 240.9366            | 1022.515            |
| Monod Kinetics |          |          |          |                     |                     |
| (2-parameter)  | -2.49014 | -191.708 | 250      | 58.82744            | 11.37712            |
| (3-parameter)  | -2.43998 | -188.452 | 236.78   | 58.63813            | 32.99903            |

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Papanastasiou,A.C.,et al (data set #1) ; Substrate : 2,4-dichlorophenoxyacetate  
Culture : activated sludge  
Condition : 20C & neutral pH

Num.pts.= 10

| Raw Data |       | Summary of results: |          |          |          |          |          |  |
|----------|-------|---------------------|----------|----------|----------|----------|----------|--|
| S(ppm)   | t(hr) | Kinetic Model       | k        | K        | So       | avg dt^2 | avg dS^2 |  |
| 96       | 0     | Zero-order          |          |          |          |          |          |  |
| 95       | 20    | (1-parameter)       | 0.472268 | ---      | 96       | 1096.443 | 244.5476 |  |
| 94       | 38    | (2-parameter)       | 0.738237 | ---      | 124.0818 | 415.5604 | 226.4779 |  |
| 86       | 64    | First-order         |          |          |          |          |          |  |
| 73       | 88    | (1-parameter)       | 0.010146 | ---      | 96       | 2379.698 | 653.5480 |  |
| 72       | 92    | (2-parameter)       | 0.019187 | ---      | 257.4675 | 761.4244 | 3649.284 |  |
| 65       | 98    | Monod Kinetics      |          |          |          |          |          |  |
| 60       | 103   | (2-parameter)       | 0.195637 | -31.7640 | 96       | 360.4122 | 213.1756 |  |
| 40       | 115   | (3-parameter)       | 0.270189 | -30.3574 | 105.4198 | 151.3207 | 168.6407 |  |
| 15       | 120   |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

data source -- Papanastasiou,A.C.,et al (data set #2) ; Substrate : glucose  
Culture : activated sludge  
Condition : 20C & neutral pH

um.pts.= 9

| Raw Data |       | Summary of results: |          |          |          |          |          |
|----------|-------|---------------------|----------|----------|----------|----------|----------|
| S(ppm)   | t(hr) | Kinetic Model       | k        | K        | So       | avg dt^2 | avg dS^2 |
| 84       | 0     | Zero-order          |          |          |          |          |          |
| 86       | 13    | (1-parameter)       | 1.419510 | ---      | 84       | 307.2612 | 619.1344 |
| 84       | 25    | (2-parameter)       | 2.578409 | ---      | 136.1234 | 82.09078 | 545.7554 |
| 81       | 32    | First-order         |          |          |          |          |          |
| 68       | 34    | (1-parameter)       | 0.052577 | ---      | 84       | 492.4814 | 1698.106 |
| 55       | 40    | (2-parameter)       | 0.107862 | ---      | 1084.495 | 119.9982 | 115511.0 |
| 29       | 43    | Monod Kinetics      |          |          |          |          |          |
| 8        | 46    | (2-parameter)       | 0.766787 | -14.4842 | 84       | 252.2095 | 428.2328 |
| 3        | 49    | (3-parameter)       | 1.507363 | -12.1246 | 116.4909 | 73.02659 | 325.7585 |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |



Culture : activated sludge

Condition : 20°C & neutral pH

D-57

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\_\_\_\_\_ + \_\_\_\_\_ = \_\_\_\_\_

Substrate: 1. 1,2-epoxy-3-methyl-4-vinylbenzene

Cultures : activated sludge

Condition on  $\beta$ : 200 is neutral, all

$$N_{\text{sub}} = 1000$$

gression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

ta source -- Radhakrishnan,I.,et al (data set #1) ; Substrate : phenol  
Culture : Bacillus cereus  
Condition : 40C & pH 7.1-7.5

m.pts.= 10

| Raw Data |       | Summary of results: |          |          |          |          |          |
|----------|-------|---------------------|----------|----------|----------|----------|----------|
| (ppm)    | t(hr) | Kinetic Model       | k        | K        | So       | avg dt^2 | avg dS^2 |
| 416      | 0     | Zero-order          |          |          |          |          |          |
| 393      | 1     | (1-parameter)       | 46.64099 | ---      | 416      | 0.245884 | 534.8923 |
| 357      | 2     | (2-parameter)       | 51.41300 | ---      | 447.4585 | 0.114899 | 303.7122 |
| 310      | 3     | First-order         |          |          |          |          |          |
| 262      | 4     | (1-parameter)       | 0.392374 | ---      | 416      | 4.924355 | 13460.28 |
| 200      | 5     | (2-parameter)       | 0.569849 | ---      | 1571.554 | 1.770865 | 163320.0 |
| 132      | 6     | Monod Kinetics      |          |          |          |          |          |
| 67       | 7     | (2-parameter)       | 44.63761 | -6.06976 | 416      | 0.235683 | ERR      |
| 20       | 8     | (3-parameter)       | 53.22250 | 4.024885 | 450.5269 | 0.112270 | 284.7610 |
| 4        | 9     |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Variable Biomass

ata source -- Radhakrishnan,I.,et al (data set #1) ; Substrate : phenol  
Culture : Bacillus cereus  
Condition : 40C & pH 7.1-7.5

um.pts.= 10

| Raw    | Data  |
|--------|-------|
| S(ppm) | t(hr) |
| 416    | 0     |
| 393    | 1     |
| 357    | 2     |
| 310    | 3     |
| 262    | 4     |
| 200    | 5     |
| 132    | 6     |
| 67     | 7     |
| 20     | 8     |
| 4      | 9     |
| NA     | NA    |
| NA     | NA    |
| NA     | NA    |
| NA     | NA    |
| NA     | NA    |
| NA     | NA    |
| NA     | NA    |
| NA     | NA    |
| NA     | NA    |
| NA     | NA    |
| NA     | NA    |
| NA     | NA    |
| NA     | NA    |
| NA     | NA    |
| NA     | NA    |

Summary of results:

| Kinetic        | Model         | ko       | K        | avg dt^2 | avg dS^2 |
|----------------|---------------|----------|----------|----------|----------|
| Zero-order     |               |          |          |          |          |
|                | (1-parameter) | 0.203006 | ---      | 0.112838 | 625.8657 |
| First-order    |               |          |          |          |          |
|                | (1-parameter) | 0.001243 | ---      | 2.619798 | 6575.016 |
| Monod Kinetics |               |          |          |          |          |
|                | (2-parameter) | 0.235515 | 29.21649 | 0.037376 | 68.85533 |

Bo = 143 ppm  
Yc = 0.609

D-61

---

data source -- Radhakrishnan,I.,et al (data set #2) ; Substrate : phenol

Culture : *Bacillus cereus*

Condition : 40C & pH 7.1-7.5

1m.pts.= 10

Summary of results:

| Raw    | Data  |
|--------|-------|
| 5(ppm) | t(hr) |

$\delta$  (ppm)                       $t$  (hr)

250 0

231 1

793 2

762 3

695 4

£35 5

565 6

490 7

400 8

300 9

NA NA

NA NA

NA NA

NA NA

NA NA

NA NA

NA NA

NA NA

NA NA

|    |    |
|----|----|
| HA | HA |
| NA | NA |

| Yes | No |
|-----|----|
| Yes | No |

|    |    |
|----|----|
| NA | NA |
| NA | NA |

|    |    |
|----|----|
| NA | NA |
| NA | NA |

|    |    |
|----|----|
| NA | NA |
| NA | NA |

|    |    |
|----|----|
| NA | NA |
| NA | NA |

NA NA

$E_O = 143 \text{ ppm}$

$$Y_C = 0.609$$

| Kinetic Model                   | ko       | K        | avg dt^2 | avg dS^2 |
|---------------------------------|----------|----------|----------|----------|
| Zero-order<br>(1-parameter)     | 0.216258 | ---      | 0.070397 | 155.6915 |
| First-order<br>(1-parameter)    | 0.000334 | ---      | 0.494467 | 1394.451 |
| Monod Kinetics<br>(2-parameter) | 0.170402 | -138.761 | 0.050227 | 150.5313 |

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Data source -- Radhakrishnan, I., et al (data set #3) ; Substrate : phenol

Condition : 30C & pH 7.1-7.5

Num.pts.= 7

D-63

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Variable Biomass

Data source -- Radhakrishnan,I.,et al (data set #3) ; Substrate : phenol  
Culture : Bacillus cereus  
Condition : 30C & pH 7.1-7.5

Num.pts.= 7

| Raw Data |         | Summary of results: |          |          |                   |
|----------|---------|---------------------|----------|----------|-------------------|
| S(ppm)   | t(hr)   | Kinetic Model       | ko       | K        | avg dt^2 avg dS^2 |
| 850      | 0       | Zero-order          |          |          |                   |
| 832      | 1       | (1-parameter)       | 0.143174 | ---      | 0.102209 99.17299 |
| 808      | 2       | First-order         |          |          |                   |
| 782      | 3       | (1-parameter)       | 0.000192 | ---      | 0.173861 156.2925 |
| 748      | 4       | Monod Kinetics      |          |          |                   |
| 715      | 5       | (2-parameter)       | 0.037633 | -580.414 | 0.011373 20.46545 |
| 655      | 6       |                     |          |          |                   |
| NA       | NA      |                     |          |          |                   |
| NA       | NA      |                     |          |          |                   |
| NA       | NA      |                     |          |          |                   |
| NA       | NA      |                     |          |          |                   |
| NA       | NA      |                     |          |          |                   |
| NA       | NA      |                     |          |          |                   |
| NA       | NA      |                     |          |          |                   |
| NA       | NA      |                     |          |          |                   |
| NA       | NA      |                     |          |          |                   |
| NA       | NA      |                     |          |          |                   |
| NA       | NA      |                     |          |          |                   |
| NA       | NA      |                     |          |          |                   |
| NA       | NA      |                     |          |          |                   |
| NA       | NA      |                     |          |          |                   |
| NA       | NA      |                     |          |          |                   |
| NA       | NA      |                     |          |          |                   |
| NA       | NA      |                     |          |          |                   |
| Bo =     | 155 ppm |                     |          |          |                   |
| Yc =     | 0.548   |                     |          |          |                   |



gression of CSTR Biodegradation Data (with respect to time) : Constant Biomass Assumed

ta source -- Radhakrishnan,I.,et al (data set #4) ; Substrate : phenol  
Culture : Bacillus cereus  
Condition : 40C & pH 7.1-7.5

n.pt3.= 10

| Raw Data |        | Summary of results: |          |          |          |          |          |
|----------|--------|---------------------|----------|----------|----------|----------|----------|
| s(ppm)   | t(hr)* | Kinetic Model       | k        | K        | So       | avg dt^2 | avg dS^2 |
| 404      | 0      | Zero-order          |          |          |          |          |          |
| 15.7     | 1.83   | (1-parameter)       | 65.11641 | ---      | 404      | 18.67616 | 79189.70 |
| 15.7     | 2.16   | (2-parameter)       | 62.19605 | ---      | 386.5186 | 18.66826 | 72215.36 |
| 15.7     | 2.58   | First-order         |          |          |          |          |          |
| 15.7     | 3.07   | (1-parameter)       | 4.487648 | ---      | 404      | 7.582871 | 176.7144 |
| 15.7     | 3.97   | (2-parameter)       | 0.324266 | ---      | 40.23264 | 6.071859 | 13257.17 |
| 15.7     | 4.5    | Monod Kinetics      |          |          |          |          |          |
| 15.7     | 7.75   | (2-parameter)       | -67.5043 | -26.9020 | 404      | 4.518309 | 7.184395 |
| 11.2     | 12.35  | (3-parameter)       | -67.7265 | -405.345 | 405.3451 | 4.518275 | 7.364518 |
| 7        | 15.38  |                     |          |          |          |          |          |
| NA       | NA     |                     |          |          |          |          |          |
| NA       | NA     |                     |          |          |          |          |          |
| NA       | NA     |                     |          |          |          |          |          |
| NA       | NA     |                     |          |          |          |          |          |
| NA       | NA     |                     |          |          |          |          |          |
| NA       | NA     |                     |          |          |          |          |          |
| NA       | NA     |                     |          |          |          |          |          |
| NA       | NA     |                     |          |          |          |          |          |
| NA       | NA     |                     |          |          |          |          |          |
| NA       | NA     |                     |          |          |          |          |          |
| NA       | NA     |                     |          |          |          |          |          |
| NA       | NA     |                     |          |          |          |          |          |
| NA       | NA     |                     |          |          |          |          |          |
| NA       | NA     |                     |          |          |          |          |          |
| NA       | NA     |                     |          |          |          |          |          |

REFERS TO RESIDENCE TIME (V/Q)

ression of CSTR Biodegradation Data (with respect to time) : Constant Biomass Assumed  
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a source -- Radhakrishnan,I.,et al (data set #5) ; Substrate : phenol  
Culture : Bacillus cereus  
Condition : 40C & pH 7.1-7.5

.pts.= 10

| Raw Data |        | Summary of results: |  |          |          |          |                   |
|----------|--------|---------------------|--|----------|----------|----------|-------------------|
| (ppm)    | t(hr)* | Kinetic Model       |  | k        | K        | So       | avg dt^2 avg dS^2 |
| 800      | 0      | Zero-order          |  |          |          |          |                   |
| 31.4     | 1.83   | (1-parameter)       |  | 128.8841 | ---      | 800      | 18.66155 309989.3 |
| 31.4     | 2.16   | (2-parameter)       |  | 122.8688 | ---      | 763.9844 | 18.65296 281599.3 |
| 31.4     | 2.58   | First-order         |  |          |          |          |                   |
| 31.4     | 3.07   | (1-parameter)       |  | 4.496391 | ---      | 800      | 7.204958 678.2094 |
| 31.4     | 3.97   | (2-parameter)       |  | 0.345339 | ---      | 82.93864 | 5.819280 51517.85 |
| 31.4     | 4.5    | Monod Kinetics      |  |          |          |          |                   |
| 31.4     | 7.75   | (2-parameter)       |  | -150.121 | -56.5835 | 800      | 4.528569 32.97439 |
| 22       | 12.35  | (3-parameter)       |  | -150.727 | -56.5776 | 803.2767 | 4.528528 34.04328 |
| 13.5     | 15.38  |                     |  |          |          |          |                   |
| NA       | NA     |                     |  |          |          |          |                   |
| NA       | NA     |                     |  |          |          |          |                   |
| NA       | NA     |                     |  |          |          |          |                   |
| NA       | NA     |                     |  |          |          |          |                   |
| NA       | NA     |                     |  |          |          |          |                   |
| NA       | NA     |                     |  |          |          |          |                   |
| NA       | NA     |                     |  |          |          |          |                   |
| NA       | NA     |                     |  |          |          |          |                   |
| NA       | NA     |                     |  |          |          |          |                   |
| NA       | NA     |                     |  |          |          |          |                   |
| NA       | NA     |                     |  |          |          |          |                   |
| NA       | NA     |                     |  |          |          |          |                   |
| NA       | NA     |                     |  |          |          |          |                   |
| NA       | NA     |                     |  |          |          |          |                   |
| NA       | NA     |                     |  |          |          |          |                   |
| NA       | NA     |                     |  |          |          |          |                   |

EFERS TO RESIDENCE TIME (V/Q)

gression of CSTR Biodegradation Data (with respect to time) : Constant Biomass Assumed  
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ta source -- Radhakrishnan,I.,et al (data set #6) ; Substrate : phenol  
Culture : Bacillus cereus  
Condition : 40C & pH 7.1-7.5

m.pts.= 10

| Raw Data |        | Summary of results: |          |          |          |          |          |
|----------|--------|---------------------|----------|----------|----------|----------|----------|
| s(ppm)   | t(hr)* | Kinetic Model       | k        | K        | So       | avg dt^2 | avg dS^2 |
| 200      | 0      | Zero-order          |          |          |          |          |          |
| 7.8      | 1.83   | (1-parameter)       | 32.22881 | ---      | 200      | 18.64259 | 19364.00 |
| 7.8      | 2.16   | (2-parameter)       | 30.64864 | ---      | 190.5361 | 18.63305 | 17502.77 |
| 7.8      | 2.58   | First-order         |          |          |          |          |          |
| 7.8      | 3.07   | (1-parameter)       | 4.580519 | ---      | 200      | 6.483061 | 40.20607 |
| 7.8      | 3.97   | (2-parameter)       | 0.340591 | ---      | 20.10174 | 5.005720 | 3241.826 |
| 7.8      | 4.5    | Monod Kinetics      |          |          |          |          |          |
| 7.8      | 7.75   | (2-parameter)       | -37.8698 | -13.8961 | 200      | 3.700469 | 1.813562 |
| 5        | 12.35  | (3-parameter)       | -37.9921 | -13.8950 | 200.6555 | 3.700443 | 1.856339 |
| 3.3      | 15.38  |                     |          |          |          |          |          |
| NA       | NA     |                     |          |          |          |          |          |
| NA       | NA     |                     |          |          |          |          |          |
| NA       | NA     |                     |          |          |          |          |          |
| NA       | NA     |                     |          |          |          |          |          |
| NA       | NA     |                     |          |          |          |          |          |
| NA       | NA     |                     |          |          |          |          |          |
| NA       | NA     |                     |          |          |          |          |          |
| NA       | NA     |                     |          |          |          |          |          |
| NA       | NA     |                     |          |          |          |          |          |
| NA       | NA     |                     |          |          |          |          |          |
| NA       | NA     |                     |          |          |          |          |          |
| NA       | NA     |                     |          |          |          |          |          |
| NA       | NA     |                     |          |          |          |          |          |
| NA       | NA     |                     |          |          |          |          |          |
| NA       | NA     |                     |          |          |          |          |          |
| NA       | NA     |                     |          |          |          |          |          |

D-67

EFERS TO RESIDENCE TIME (V/Q)

.....

Condition : room temperature/neutral pH

8

D-68

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Culture : activated sludge

Condition : room temperature

[illegible]

\_\_\_\_\_

Condition : 22C & neutral pH

D-70

ma.pts.= 5

D-71

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Substrate : 3,5-dichlorobenzoate

6

Condition : 20C & neutral pH

8

D-72



.....

Substrate : 3,5-dichlorobenzoate

Condition : 20C & neutral pH

C17

D-73

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Tanner,R.D.,et al (data set #1) ;

Substrate : glucose

Culture : pseudomonas ovalis

Condition : room temperature/neutral pH

Num.pts.= 11

| Raw    | Data  |
|--------|-------|
| S(ppm) | t(hr) |
| 51833  | 0     |
| 50802  | 1     |
| 49541  | 2     |
| 48280  | 3     |
| 46118  | 4     |
| 41434  | 5     |
| 30085  | 6     |
| 17907  | 7     |
| 7404   | 8     |
| 2396   | 9     |
| 1250   | 10    |
| NA     | NA    |
| NA     | NA    |
| NA     | NA    |
| NA     | NA    |
| NA     | NA    |
| NA     | NA    |
| NA     | NA    |
| NA     | NA    |
| NA     | NA    |
| NA     | NA    |
| NA     | NA    |
| NA     | NA    |
| NA     | NA    |
| NA     | NA    |
| NA     | NA    |
| NA     | NA    |

Summary of results:

| Kinetic Model  | k        | K        | So       | avg dt^2 | avg dS^2 |
|----------------|----------|----------|----------|----------|----------|
| Zero-order     |          |          |          |          |          |
| (1-parameter)  | 4962.506 | ---      | 51833    | 2.661244 | 65537053 |
| (2-parameter)  | 6517.919 | ---      | 64139.59 | 0.937864 | 39843539 |
| First-order    |          |          |          |          |          |
| (1-parameter)  | 0.307299 | ---      | 51833    | 7.458280 | 3.5E-08  |
| (2-parameter)  | 0.460764 | ---      | 193909.9 | 2.314333 | 2.5E-09  |
| Monod Kinetics |          |          |          |          |          |
| (2-parameter)  | 3676.869 | -4746.80 | 51833    | 2.280213 | ERR      |
| (3-parameter)  | 5776.205 | -1864.47 | 62619    | 0.917280 | ERR      |

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Substrate : glucose  
Culture : *pseudomonas ovalis*  
Condition : room temperature/neutral pH

Num.pts. = 11

Bo = 0.108 optical units  
Yc = 0.00005 optical unit/ppm

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Substrate : o-phthalic acid  
Culture : activated sludge  
Condition : 30C & neutral pH

Num.pts.= 6

[illegible]

Substrate : o-phthalic acid  
Culture : activated sludge  
Condition : 30C & neutral pH

Substrate : o-phthalic acid  
Culture : activated sludge  
Condition : 30C & neutral pH

D-77

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Substrate : o-phthalic acid  
Culture : activated sludge  
Condition : 30C & neutral pH

Substrate : o-phthalic acid  
Culture : activated sludge  
Condition : 30C & neutral pH

D-78

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Data source -- Wong,P.T.S. and Kaiser,K.L.E. (data set #1) ; Substrate : 4-chlorobiphenyl  
Culture : acclimated Lake Ontario  
Condition : room temperature/neutra

Num.pts.= 4

[illegible]

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Num.pts.= 4

D-80



gression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

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ata source -- Wong,P.T.S. and Kaiser,K.L.E. (data set #3) ; Substrate : biphenyl
Culture      : acclimated Lake Ontario bacteria
Condition   : room temperature/neutral pH
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im.pts.= 4

[illegible]

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Num.pts.= 6

D-82

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Num.pts.= 6

Bo = 0.0012 ppm  
Yc = 0.1

D-83

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Yordy,J.R.,et al (data set #1) ; Substrate : N-nitrosodiethanolamine  
Culture : Canyon Lake bacteria  
Condition : 22C & pH 7.8

Num.pts.= 20

| Raw Data |       | Summary of results: |          |          |          |          |          |
|----------|-------|---------------------|----------|----------|----------|----------|----------|
| S(ppm)   | t(hr) | Kinetic Model       | k        | K        | So       | avg dt^2 | avg dS^2 |
| 1        | 0     | Zero-order          |          |          |          |          |          |
| 0.97     | 24    | (1-parameter)       | 0.002141 | ---      | 1        | 7001.852 | 0.032102 |
| 0.99     | 48    | (2-parameter)       | 0.002875 | ---      | 1.283511 | 2023.515 | 0.016733 |
| 1.09     | 72    | First-order         |          |          |          |          |          |
| 1.04     | 96    | (1-parameter)       | 0.008966 | ---      | 1        | 18304.64 | 0.199257 |
| 1.01     | 120   | (2-parameter)       | 0.013552 | ---      | 6.857918 | 5148.531 | 3.043739 |
| 0.89     | 144   | Monod Kinetics      |          |          |          |          |          |
| 0.93     | 168   | (2-parameter)       | 0.001925 | -0.02797 | 1        | 6869.270 | ERR      |
| 0.92     | 192   | (3-parameter)       | 0.003148 | 0.024228 | 1.3105   | 1988.552 | 0.017174 |
| 0.8      | 216   |                     |          |          |          |          |          |
| 0.74     | 240   |                     |          |          |          |          |          |
| 0.61     | 264   |                     |          |          |          |          |          |
| 0.41     | 312   |                     |          |          |          |          |          |
| 0.26     | 336   |                     |          |          |          |          |          |
| 0.13     | 360   |                     |          |          |          |          |          |
| 0.1      | 384   |                     |          |          |          |          |          |
| 0.02     | 408   |                     |          |          |          |          |          |
| 0.014    | 432   |                     |          |          |          |          |          |
| 0.007    | 456   |                     |          |          |          |          |          |
| 0.005    | 504   |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Yordy,J.R.,et al (data set #2) ;

Substrate : N-nitrosodiethanolamine  
Culture : North Lake bacteria  
Condition : 22C & pH 7.8

Num.pts.= 17

| Raw    | Data  | Summary of results: |       |          |          |          |                   |
|--------|-------|---------------------|-------|----------|----------|----------|-------------------|
| S(ppm) | t(hr) | Kinetic             | Model | k        | K        | So       | avg dt^2 avg dS^2 |
| 1      | 0     | Zero-order          |       |          |          |          |                   |
| 1      | 24    | (1-parameter)       |       | 0.001655 | ---      | 1        | 11113.74 0.030466 |
| 0.94   | 72    | (2-parameter)       |       | 0.002255 | ---      | 1.266651 | 3512.063 0.017874 |
| 1.01   | 96    | First-order         |       |          |          |          |                   |
| 1      | 120   | (1-parameter)       |       | 0.005763 | ---      | 1        | 27202.95 0.171877 |
| 0.94   | 168   | (2-parameter)       |       | 0.008757 | ---      | 4.345570 | 7687.769 1.253297 |
| 0.96   | 192   | Monod Kinetics      |       |          |          |          |                   |
| 0.91   | 240   | (2-parameter)       |       | 0.001169 | -0.09805 | 1        | 9411.287 ERR      |
| 0.79   | 264   | (3-parameter)       |       | 0.001961 | -0.03911 | 1.2301   | 3429.460 ERR      |
| 0.79   | 288   |                     |       |          |          |          |                   |
| 0.71   | 312   |                     |       |          |          |          |                   |
| 0.54   | 336   |                     |       |          |          |          |                   |
| 0.4    | 384   |                     |       |          |          |          |                   |
| 0.22   | 432   |                     |       |          |          |          |                   |
| 0.04   | 480   |                     |       |          |          |          |                   |
| 0.03   | 528   |                     |       |          |          |          |                   |
| 0.02   | 600   |                     |       |          |          |          |                   |
| NA     | NA    |                     |       |          |          |          |                   |
| NA     | NA    |                     |       |          |          |          |                   |
| NA     | NA    |                     |       |          |          |          |                   |
| NA     | NA    |                     |       |          |          |          |                   |
| NA     | NA    |                     |       |          |          |          |                   |
| NA     | NA    |                     |       |          |          |          |                   |
| NA     | NA    |                     |       |          |          |          |                   |
| NA     | NA    |                     |       |          |          |          |                   |

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

ata source -- Yordy,J.R.,et al (data set #3) ; Substrate : N-nitrosodiethanolamine  
Culture : Canyon Lake bacteria  
Condition : 22C & pH 7.8

um.pts.= 14

| Raw    | Data  | Summary of results: |       |   |   |    |                   |
|--------|-------|---------------------|-------|---|---|----|-------------------|
| S(ppm) | t(hr) | Kinetic             | Model | k | K | So | avg dt^2 avg dS^2 |
| 0.05   | 0     | Zero-order          |       |   |   |    |                   |
| 0.049  | 24    | (1-parameter)       |       |   |   |    |                   |
| 0.05   | 48    | (2-parameter)       |       |   |   |    |                   |
| 0.051  | 72    | First-order         |       |   |   |    |                   |
| 0.049  | 96    | (1-parameter)       |       |   |   |    |                   |
| 0.028  | 120   | (2-parameter)       |       |   |   |    |                   |
| 0.024  | 144   | Monod Kinetics      |       |   |   |    |                   |
| 0.008  | 168   | (2-parameter)       |       |   |   |    |                   |
| 0.009  | 192   | (3-parameter)       |       |   |   |    |                   |
| 0.014  | 216   |                     |       |   |   |    |                   |
| 0.004  | 240   |                     |       |   |   |    |                   |
| 0.001  | 264   |                     |       |   |   |    |                   |
| 0.003  | 288   |                     |       |   |   |    |                   |
| 0.001  | 312   |                     |       |   |   |    |                   |
| NA     | NA    |                     |       |   |   |    |                   |
| NA     | NA    |                     |       |   |   |    |                   |
| NA     | NA    |                     |       |   |   |    |                   |
| NA     | NA    |                     |       |   |   |    |                   |
| NA     | NA    |                     |       |   |   |    |                   |
| NA     | NA    |                     |       |   |   |    |                   |
| NA     | NA    |                     |       |   |   |    |                   |
| NA     | NA    |                     |       |   |   |    |                   |
| NA     | NA    |                     |       |   |   |    |                   |
| NA     | NA    |                     |       |   |   |    |                   |
| NA     | NA    |                     |       |   |   |    |                   |

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Yordy,J.R.,et al (data set #4) ; Substrate : N-nitrosodiethanolamine  
Culture : Canyon Lake bacteria  
Condition : 22C & pH 7.8

Num.pts.= 15

| Raw Data |       | Summary of results: |          |          |          |          |          |  |
|----------|-------|---------------------|----------|----------|----------|----------|----------|--|
| S(ppm)   | t(hr) | Kinetic Model       | k        | K        | So       | avg dt^2 | avg dS^2 |  |
| 0.05     | 0     | Zero-order          |          |          |          |          |          |  |
| 0.047    | 24    | (1-parameter)       | 0.000169 | ---      | 0.05     | 2330.840 | 0.000067 |  |
| 0.05     | 48    | (2-parameter)       | 0.000214 | ---      | 0.061213 | 1190.683 | 0.000054 |  |
| 0.051    | 72    | First-order         |          |          |          |          |          |  |
| 0.049    | 96    | (1-parameter)       | 0.011330 | ---      | 0.05     | 4586.443 | 0.000286 |  |
| 0.047    | 120   | (2-parameter)       | 0.015842 | ---      | 0.168864 | 1473.412 | 0.001375 |  |
| 0.029    | 144   | Monod Kinetics      |          |          |          |          |          |  |
| 0.025    | 168   | (2-parameter)       | 0.000190 | 0.002018 | 0.05     | 2291.707 | 0.000068 |  |
| 0.009    | 192   | (3-parameter)       | 0.000347 | 0.009202 | 0.0675   | 960.4635 | 0.000060 |  |
| 0.011    | 216   |                     |          |          |          |          |          |  |
| 0.004    | 240   |                     |          |          |          |          |          |  |
| 0.001    | 264   |                     |          |          |          |          |          |  |
| 0.003    | 288   |                     |          |          |          |          |          |  |
| 0.001    | 312   |                     |          |          |          |          |          |  |
| 0.001    | 336   |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |

gression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

ata source -- Yordy,J.R.,et al (data set #5) ; Substrate : N-nitrosodiethanolamine  
Culture : Canyon Lake bacteria  
Condition : 22C & pH 7.8

um.pts.= 25

| Raw Data |       | Summary of results: |          |          |          |          |          |
|----------|-------|---------------------|----------|----------|----------|----------|----------|
| S(ppm)   | t(hr) | Kinetic Model       | k        | K        | So       | avg dt^2 | avg dS^2 |
| 0.045    | 0     | Zero-order          |          |          |          |          |          |
| 0.045    | 24    | (1-parameter)       | 0.000072 | ---      | 0.045    | 23845.07 | 0.000124 |
| 0.04     | 48    | (2-parameter)       | 0.000109 | ---      | 0.063223 | 6768.866 | 0.000081 |
| 0.046    | 72    | First-order         |          |          |          |          |          |
| 0.046    | 96    | (1-parameter)       | 0.008753 | ---      | 0.045    | 49546.44 | 0.000696 |
| 0.046    | 120   | (2-parameter)       | 0.014691 | ---      | 1.086374 | 13478.09 | 0.081610 |
| 0.045    | 144   | Monod Kinetics      |          |          |          |          |          |
| 0.046    | 168   | (2-parameter)       | 0.000058 | -0.00206 | 0.045    | 22635.72 | 0.000078 |
| 0.046    | 192   | (3-parameter)       | 0.000102 | -0.00065 | 0.062    | 6730.221 | ERR      |
| 0.046    | 216   |                     |          |          |          |          |          |
| 0.044    | 240   |                     |          |          |          |          |          |
| 0.039    | 264   |                     |          |          |          |          |          |
| 0.045    | 288   |                     |          |          |          |          |          |
| 0.037    | 312   |                     |          |          |          |          |          |
| 0.04     | 336   |                     |          |          |          |          |          |
| 0.039    | 360   |                     |          |          |          |          |          |
| 0.022    | 384   |                     |          |          |          |          |          |
| 0.023    | 408   |                     |          |          |          |          |          |
| 0.017    | 432   |                     |          |          |          |          |          |
| 0.02     | 456   |                     |          |          |          |          |          |
| 0.004    | 480   |                     |          |          |          |          |          |
| 0.003    | 504   |                     |          |          |          |          |          |
| 0.0001   | 528   |                     |          |          |          |          |          |
| 0.0001   | 576   |                     |          |          |          |          |          |
| 0.0001   | 624   |                     |          |          |          |          |          |



egression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

ata source -- Yordy,J.R.,et al (data set #6) ; Substrate : N-nitrosodiethanolamine  
 Culture : sewage  
 Condition : 22C & pH 7.8

um.pts.= 25

| Raw Data |       | Summary of results: |          |          |          |          |          |  |
|----------|-------|---------------------|----------|----------|----------|----------|----------|--|
| S(ppm)   | t(hr) | Kinetic Model       | k        | K        | So       | avg dt^2 | avg dS^2 |  |
| 1        | 0     | Zero-order          |          |          |          |          |          |  |
| 0.95     | 24    | (1-parameter)       | 0.001147 | ---      | 1        | 7559.095 | 0.009953 |  |
| 1        | 72    | (2-parameter)       | 0.001407 | ---      | 1.157833 | 2779.628 | 0.005504 |  |
| 1.03     | 120   | First-order         |          |          |          |          |          |  |
| 1        | 144   | (1-parameter)       | 0.003046 | ---      | 1        | 36075.43 | 0.067779 |  |
| 0.93     | 192   | (2-parameter)       | 0.004507 | ---      | 2.665134 | 9855.020 | 0.261582 |  |
| 0.89     | 216   | Monod Kinetics      |          |          |          |          |          |  |
| 0.83     | 264   | (2-parameter)       | 0.001011 | -0.05036 | 1        | 7105.522 | ERR      |  |
| 0.79     | 312   | (3-parameter)       | 0.001533 | 0.032263 | 1.176    | 2712.667 | 0.005628 |  |
| 0.77     | 336   |                     |          |          |          |          |          |  |
| 0.67     | 384   |                     |          |          |          |          |          |  |
| 0.65     | 408   |                     |          |          |          |          |          |  |
| 0.58     | 432   |                     |          |          |          |          |          |  |
| 0.44     | 456   |                     |          |          |          |          |          |  |
| 0.56     | 480   |                     |          |          |          |          |          |  |
| 0.48     | 504   |                     |          |          |          |          |          |  |
| 0.44     | 528   |                     |          |          |          |          |          |  |
| 0.32     | 552   |                     |          |          |          |          |          |  |
| 0.26     | 576   |                     |          |          |          |          |          |  |
| 0.21     | 600   |                     |          |          |          |          |          |  |
| 0.14     | 672   |                     |          |          |          |          |          |  |
| 0.11     | 744   |                     |          |          |          |          |          |  |
| 0.06     | 792   |                     |          |          |          |          |          |  |
| 0.05     | 814   |                     |          |          |          |          |          |  |
| 0.03     | 864   |                     |          |          |          |          |          |  |

Appendix E

Compilation of Regression Analysis Results for Aerobic

Biodegradation Data from Previous NJIT MS Theses

Table of Contents

|  | <u>Page</u>  |
|--|--------------|
| List of MS Theses  | E-3          |
| Index of Batch Reactor Data Analysis Results   | E-4          |
| Regression Analysis Results (for above MS Theses,<br>provided in alphabetical order) | E-6 to E-108 |

List of MS Theses

1. Colish, J., "Biodegradation of Phenol and o-Chlorophenol Using Activated Sludge Bacteria," MS Thesis, New Jersey Institute of Technology (1984).
2. Gonnaphula, P., "Biodegradation of Mixed Phenolic Substrates," New Jersey Institute of Technology (1986).
3. McMullen, N., "A Comparison of the Biodegradation of Phenol and o-Chlorophenol Using a Municipal Mixed Liquor and Three Commercial Microbial Populations," New Jersey Institute of Technology (1985).
4. Naik, N., "Biodegradation of Multiple Substrates in a Batch Reactor," New Jersey Institute of Technology (1986).
5. Pak, K., "Biodegradation of Phenolics Using Mixed Liquor from Passaic Valley Sewerage Commissioner's Plant (Newark, NJ)," New Jersey Institute of Technology (1985).
6. Salerno, S., "A Comparison of the Biodegradation of Nitrobenzene, 1-Butanol and 2,4-Dichlorophenoxyacetic Acid Using a Municipal Mixed Liquor and Three Commercial Microbial Populations," New Jersey Institute of Technology (1984).

Index of Batch Reactor Data Analysis Results

| <u>MS Thesis</u> | <u>Substrate</u>    | <u>Medium</u>    | <u>Biomass<br/>Type</u> | <u># Sets</u> | <u>Page</u>  |
|------------------|---------------------|------------------|-------------------------|---------------|--|
| 1                | Phenol              | Activated sludge | Constant                | 1             | E-6  |
|                  |                     |                  | Variable                | 1             | E-7  |
|                  | 2-chlorophenol      | Activated sludge | Constant                | 6             | E-8, E-10,<br>E-12, E-14,<br>E-16, E-18  |
|                  |                     |                  | Variable                | 6             | E-9, E-11,<br>E-13, E-15,<br>E-17, E-19  |
| 2                | Phenol              | Activated sludge | Constant                | 14            | E-20, E-22,<br>E-24, E-26,<br>E-28, E-30,<br>E-32, E-34,<br>E-36, E-38,<br>E-40, E-42,<br>E-44, E-46 |
|                  |                     |                  |                         |               |  |
|                  |                     |                  |                         |               |  |
|                  |                     |                  |                         |               |  |
|                  | 2,6-dichloro-phenol | Activated sludge | Constant                | 5             | E-21, E-23,<br>E-25, E-27,<br>E-29   |
|                  | 2-chlorophenol      | Activated sludge | Constant                | 5             | E-31, E-33,<br>E-35, E-37,<br>E-39   |
|                  | Nitrobenzene        | Activated sludge | Constant                | 4             | E-41, E-43,<br>E-45, E-47  |
|                  |                     |                  |                         |               |  |
| 3                | Phenol              | Activated sludge | Constant                | 2             | E-48, E-50   |
|                  |                     |                  | Variable                | 2             | E-49, E-51   |
|                  | 2-chlorophenol      | Activated sludge | Constant                | 3             | E-52, E-54,<br>E-56  |
|                  |                     |                  | Variable                | 3             | E-53, E-55,<br>E-57  |

| <u>MS Thesis</u> | <u>Substrate</u>    | <u>Medium</u>    | <u>Biomass Type</u> | <u># Sets</u> | <u>Page</u>   |
|------------------|---------------------|------------------|---------------------|---------------|---|
| 4                | Phenol              | Activated sludge | Constant            | 6             | E-58, E-61,<br>E-64, E-67,<br>E-70, E-73  |
|                  | 2-chlorophenol      | Activated sludge | Constant            | 4             | E-76, E-79,<br>E-82, E-85   |
|                  | Nitrobenzene        | Activated sludge | Constant            | 12            | E-59, E-62,<br>E-65, E-68,<br>E-71, E-74,<br>E-77, E-80,<br>E-83, E-86,<br>E-88, E-90 |
|                  | 2,6-dichloro-phenol | Activated sludge | Constant            | 12            | E-60, E-63,<br>E-66, E-69,<br>E-72, E-75,<br>E-78, E-81,<br>E-84, E-87,<br>E-89, E-91 |
| 5                | 2,6-dichloro-phenol | Activated sludge | Constant            | 4             | E-92, E-94,<br>E-95, E-97   |
|                  |                     |                  | Variable            | 2             | E-93, E-96  |
|                  | 2-chlorophenol      | Activated sludge | Constant            | 4             | E-98, E-100,<br>E-101, E-103  |
|                  |                     |                  | Variable            | 2             | E-99, E-102   |
| 6                | Phenol              | Activated sludge | Constant            | 2             | E-104, E-106  |
|                  |                     |                  | Variable            | 1             | E-105   |
|                  | 2,4-dichloro-phenol | Activated sludge | Constant            | 1             | E-107   |
|                  |                     |                  | Variable            | 1             | E-108   |

-----

Substrate : phenol  
Culture : mssa  
Condition : room temperature & pH 6.9

Num.pts.= 7

[illegible]

\* corresponds to data extracted from Table 20 on page 92.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Variable Biomass

data source -- Colish Thesis (data set #1)\*; Substrate : phenol  
Culture : mls Culture : mls  
Condition : room temperature & pH 6.9

pts.= 7

| Raw Data |           | Summary of results: |          |          |                   |
|----------|-----------|---------------------|----------|----------|-------------------|
| S(ppm)   | t(hr)     | Kinetic Model       | ko       | K        | avg dt^2 avg dS^2 |
| 33.687   | 0         | Zero-order          |          |          |                   |
| 21.007   | 0.333     | (1-parameter)       | 0.061106 | ---      | 0.016304 64.89691 |
| 03.234   | 0.667     | First-order         |          |          |                   |
| 91.888   | 1         | (1-parameter)       | 0.000892 | ---      | 0.072210 319.4442 |
| 43.417   | 1.333     | Monod Kinetics      |          |          |                   |
| 31.503   | 1.667     | (2-parameter)       | 0.058391 | -3.16082 | 0.016189 73.95568 |
| 15.27    | 2         |                     |          |          |                   |
| NA       | NA        |                     |          |          |                   |
| NA       | NA        |                     |          |          |                   |
| NA       | NA        |                     |          |          |                   |
| NA       | NA        |                     |          |          |                   |
| NA       | NA        |                     |          |          |                   |
| NA       | NA        |                     |          |          |                   |
| NA       | NA        |                     |          |          |                   |
| NA       | NA        |                     |          |          |                   |
| NA       | NA        |                     |          |          |                   |
| NA       | NA        |                     |          |          |                   |
| NA       | NA        |                     |          |          |                   |
| NA       | NA        |                     |          |          |                   |
| NA       | NA        |                     |          |          |                   |
| NA       | NA        |                     |          |          |                   |
| NA       | NA        |                     |          |          |                   |
| NA       | NA        |                     |          |          |                   |
| NA       | NA        |                     |          |          |                   |
| NA       | NA        |                     |          |          |                   |
| Bo =     | 811 ppm** |                     |          |          |                   |
| Yc =     | 3.51**    |                     |          |          |                   |

\* corresponds to data extracted from Table 20 on page 92.  
\*\*estimated from available MLSS measurements.



.....

Substrate : o-chlorophenol  
Culture : mlss  
Condition : room temperature & pH 7.0

Num.pts.\* 8

[illegible]

\* corresponds to data extracted from Table 21 on page 93.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Variable Biomass  
-----

Data source -- Colish Thesis (data set #2)\*;                      Substrate : o-chlorophenol  
   Culture    : mlss  
   Condition : room temperature & pH 7.0

Num.pts.=                      8

| Raw Data |            | Summary of results: |          |          |          |          |
|----------|------------|---------------------|----------|----------|----------|----------|
| S(ppm)   | t(hr)      | Kinetic Model       | ko       | K        | avg dt^2 | avg dS^2 |
| 19.584   | 0          | Zero-order          |          |          |          |          |
| 17.922   | 1          | (1-parameter)       | 0.001272 | ---      | 0.359394 | 1.887232 |
| 18.192   | 2          | First-order         |          |          |          |          |
| 13.758   | 3          | (1-parameter)       | 0.000132 | ---      | 1.829427 | 10.55572 |
| 11.853   | 4          | Monod Kinetics      |          |          |          |          |
| 7.523    | 5          | (2-parameter)       | 0.000972 | -2.43761 | 0.267972 | ERR      |
| 6.042    | 6          |                     |          |          |          |          |
| 2.319    | 7          |                     |          |          |          |          |
| NA       | NA         |                     |          |          |          |          |
| NA       | NA         |                     |          |          |          |          |
| NA       | NA         |                     |          |          |          |          |
| NA       | NA         |                     |          |          |          |          |
| NA       | NA         |                     |          |          |          |          |
| NA       | NA         |                     |          |          |          |          |
| NA       | NA         |                     |          |          |          |          |
| NA       | NA         |                     |          |          |          |          |
| NA       | NA         |                     |          |          |          |          |
| NA       | NA         |                     |          |          |          |          |
| NA       | NA         |                     |          |          |          |          |
| NA       | NA         |                     |          |          |          |          |
| NA       | NA         |                     |          |          |          |          |
| NA       | NA         |                     |          |          |          |          |
| NA       | NA         |                     |          |          |          |          |
| NA       | NA         |                     |          |          |          |          |
| NA       | NA         |                     |          |          |          |          |
| Bo =     | 1780 ppm** |                     |          |          |          |          |
| Yc =     | 4.05**     |                     |          |          |          |          |

\* corresponds to data extracted from Table 21 on page 93.  
\*\*estimated from available MLSS measurements.

.....

Condition : room temperature & pH 7.0-7.5

5

E-10

\* corresponds to data extracted from Table 22 on page 94.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Variable Biomass

Data source -- Colish Thesis (data set #3) \*; Substrate : o-chlorophenol  
Culture : mlss  
Condition : room temperature & pH 7.0-7.5

Num.pts.= 5

| Raw Data |             | Summary of results: |          |          |          |          |
|----------|-------------|---------------------|----------|----------|----------|----------|
| S(ppm)   | t(hr)       | Kinetic Model       | ko       | K        | avg dt^2 | avg dS^2 |
| 19.121   | 0           | Zero-order          |          |          |          |          |
| 15.922   | 1           | (1-parameter)       | 0.002865 | ---      | 0.024874 | 0.519680 |
| 10.561   | 2           | First-order         |          |          |          |          |
| 4.582    | 3           | (1-parameter)       | 0.000400 | ---      | 0.525563 | 12.88930 |
| 0.915    | 4           | Monod Kinetics      |          |          |          |          |
| NA       | NA          | (2-parameter)       | 0.002857 | -0.01946 | 0.024871 | 0.520128 |
| NA       | NA          |                     |          |          |          |          |
| NA       | NA          |                     |          |          |          |          |
| NA       | NA          |                     |          |          |          |          |
| NA       | NA          |                     |          |          |          |          |
| NA       | NA          |                     |          |          |          |          |
| NA       | NA          |                     |          |          |          |          |
| NA       | NA          |                     |          |          |          |          |
| NA       | NA          |                     |          |          |          |          |
| NA       | NA          |                     |          |          |          |          |
| NA       | NA          |                     |          |          |          |          |
| NA       | NA          |                     |          |          |          |          |
| NA       | NA          |                     |          |          |          |          |
| NA       | NA          |                     |          |          |          |          |
| NA       | NA          |                     |          |          |          |          |
| NA       | NA          |                     |          |          |          |          |
| NA       | NA          |                     |          |          |          |          |
| NA       | NA          |                     |          |          |          |          |
| NA       | NA          |                     |          |          |          |          |
| Bo =     | 1540 ppm ** |                     |          |          |          |          |
| Yc =     | 7.57 **     |                     |          |          |          |          |

\* corresponds to data extracted from Table 22 on page 94.  
\*\*estimated from available MLSS measurements.

---

Substrate : o-chlorophenol  
Culture : m1ss  
Condition : room temperature & pH 6.9-7.0

Condition : room temperature & pH 6.9-7.0

E-12

\* corresponds to data extracted from Table 23 on page 95.

.....

Substrate : o-chlorophenol  
Culture : m1ss  
Condition : room temperature & pH 6.9-7.0

Num.pts.= 4

[illegible]

\*\*estimated from available MLSS measurements.

-----

Data source -- Colish Thesis (data set #5) \*

Substrate : o-chlorophenol  
Culture : m1ss  
Condition : room temperature & pH 7.3-7.8

Num.pts.= 14

[illegible]

E-14

\* corresponds to data extracted from Table 24 on page 96.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Variable Biomass

Data source -- Colish Thesis (data set #5)\*;

Substrate : o-chlorophenol

Culture : mlss

Condition : room temperature & pH 6.9-7.0

Num.pts.= 14

| Raw    | Data  |
|--------|-------|
| S(ppm) | t(hr) |
| 36.927 | 0     |
| 37.568 | 0.5   |
| 38.144 | 1     |
| 36.131 | 1.5   |
| 33.3   | 2     |
| 30.978 | 2.5   |
| 28.965 | 3     |
| 23.106 | 4     |
| 20.916 | 4.5   |
| 14.635 | 5     |
| 11.547 | 5.5   |
| 7.678  | 6     |
| 2.461  | 6.5   |
| 0.385  | 7     |
| NA     | NA    |
| NA     | NA    |
| NA     | NA    |
| NA     | NA    |
| NA     | NA    |
| NA     | NA    |
| NA     | NA    |
| NA     | NA    |
| NA     | NA    |
| NA     | NA    |
| NA     | NA    |
| NA     | NA    |

Summary of results:

| Kinetic Model  | ko       | K        | avg dt^2 | avg dS^2 |
|----------------|----------|----------|----------|----------|
| Zero-order     |          |          |          |          |
| (1-parameter)  | 0.005770 | ---      | 0.816730 | 17.66430 |
| First-order    |          |          |          |          |
| (1-parameter)  | 0.000521 | ---      | 4.780547 | 158.1892 |
| Monod Kinetics |          |          |          |          |
| (2-parameter)  | 0.004724 | -2.52899 | 0.653413 | 14.34113 |

Bo = 780 ppm \*\*  
Yc = 2.38 \*\*

\* corresponds to data extracted from Table 24 on page 96.

\*\* estimated from available MLSS measurements.



Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

data source -- Colish Thesis (data set #6)\*;

Substrate : o-chlorophenol  
 Culture : mlss  
 Condition : room temperature & pH 7.0-7.3

lum.pts.= 20

| Raw Data |       | Summary of results: |  |          |          |          |          |          |
|----------|-------|---------------------|--|----------|----------|----------|----------|----------|
| S(ppm)   | t(hr) | Kinetic Model       |  | k        | K        | So       | avg dt^2 | avg dS^2 |
| 39.764   | 0     | Zero-order          |  |          |          |          |          |          |
| 43.189   | 0.5   | (1-parameter)       |  | 3.137690 | ---      | 39.764   | 1.601205 | 15.76403 |
| 37.345   | 1     | (2-parameter)       |  | 3.969826 | ---      | 46.21755 | 0.467145 | 7.361992 |
| 37.795   | 1.5   | First-order         |  |          |          |          |          |          |
| 37.84    | 2     | (1-parameter)       |  | 0.222962 | ---      | 39.764   | 10.73131 | 131.1092 |
| 36.375   | 2.5   | (2-parameter)       |  | 0.365603 | ---      | 133.7009 | 3.566880 | 987.7162 |
| 35.582   | 3.5   | Monod Kinetics      |  |          |          |          |          |          |
| 34.108   | 4     | (2-parameter)       |  | 2.536906 | -3.47718 | 39.764   | 1.172813 | 12.13608 |
| 32.016   | 4.5   | (3-parameter)       |  | 3.356384 | -2.37681 | 44.937   | 0.365404 | 5.366433 |
| 28.447   | 5     |                     |  |          |          |          |          |          |
| 27.311   | 5.5   |                     |  |          |          |          |          |          |
| 24.139   | 6     |                     |  |          |          |          |          |          |
| 21.793   | 6.5   |                     |  |          |          |          |          |          |
| 19.779   | 7     |                     |  |          |          |          |          |          |
| 17.066   | 7.5   |                     |  |          |          |          |          |          |
| 14.474   | 8     |                     |  |          |          |          |          |          |
| 11.968   | 8.5   |                     |  |          |          |          |          |          |
| 10.338   | 9     |                     |  |          |          |          |          |          |
| 7.365    | 9.5   |                     |  |          |          |          |          |          |
| 0.75     | 10.5  |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |

\* corresponds to data extracted from Table 25 on page 97.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Variable Biomass

Data source -- Colish Thesis (data set #6)\*;

Substrate : o-chlorophenol  
Culture : mlss  
Condition : room temperature & pH 7.0-7.3

Num.pts.= 20

| Raw Data |         | Summary of results: |          |          |          |          |
|----------|---------|---------------------|----------|----------|----------|----------|
| S(ppm)   | t(hr)   | Kinetic Model       | ko       | K        | avg dt^2 | avg dS^2 |
| 39.764   | 0       | Zero-order          |          |          |          |          |
| 43.189   | 0.5     | (1-parameter)       | 0.004078 | ---      | 1.447083 | 14.01920 |
| 37.345   | 1       | First-order         |          |          |          |          |
| 37.795   | 1.5     | (1-parameter)       | 0.000275 | ---      | 9.981147 | 118.8475 |
| 37.84    | 2       | Monod Kinetics      |          |          |          |          |
| 36.375   | 2.5     | (2-parameter)       | 0.003339 | -3.39594 | 1.094488 | 10.91781 |
| 35.582   | 3.5     |                     |          |          |          |          |
| 34.108   | 4       |                     |          |          |          |          |
| 32.016   | 4.5     |                     |          |          |          |          |
| 28.447   | 5       |                     |          |          |          |          |
| 27.311   | 5.5     |                     |          |          |          |          |
| 24.139   | 6       |                     |          |          |          |          |
| 21.793   | 6.5     |                     |          |          |          |          |
| 19.779   | 7       |                     |          |          |          |          |
| 17.066   | 7.5     |                     |          |          |          |          |
| 14.474   | 8       |                     |          |          |          |          |
| 11.968   | 8.5     |                     |          |          |          |          |
| 10.338   | 9       |                     |          |          |          |          |
| 7.365    | 9.5     |                     |          |          |          |          |
| 0.75     | 10.5    |                     |          |          |          |          |
| NA       | NA      |                     |          |          |          |          |
| NA       | NA      |                     |          |          |          |          |
| NA       | NA      |                     |          |          |          |          |
| NA       | NA      |                     |          |          |          |          |
| NA       | NA      |                     |          |          |          |          |
| Bo =     | 730 ppm |                     |          |          |          |          |
| Yc =     | 2.74 ** |                     |          |          |          |          |

\* corresponds to data extracted from Table 25 on page 97.

\*\*estimated from available MLSS measurements.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Colish Thesis (data set #7)\*; Substrate : o-chlorophenol  
Culture : mls Culture : mls  
Condition : room temperature & pH 7.0-7.3

Num.pts.= 15

| Raw Data |       | Summary of results: |          |          |          |          |          |  |
|----------|-------|---------------------|----------|----------|----------|----------|----------|--|
| S(ppm)   | t(hr) | Kinetic Model       | k        | K        | So       | avg dt^2 | avg dS^2 |  |
| 39.665   | 0     | Zero-order          |          |          |          |          |          |  |
| 36.011   | 0.5   | (1-parameter)       | 5.027012 | ---      | 39.665   | 0.767499 | 19.39536 |  |
| 37.724   | 1     | (2-parameter)       | 6.276865 | ---      | 46.26842 | 0.301037 | 11.86059 |  |
| 37.165   | 1.5   | First-order         |          |          |          |          |          |  |
| 39.422   | 2     | (1-parameter)       | 0.343322 | ---      | 39.665   | 3.619149 | 124.5127 |  |
| 34.92    | 2.5   | (2-parameter)       | 0.523687 | ---      | 112.7548 | 1.216559 | 624.1664 |  |
| 29.626   | 3     | Monod Kinetics      |          |          |          |          |          |  |
| 27.539   | 3.5   | (2-parameter)       | 4.033279 | -3.39825 | 39.665   | 0.635152 | ERR      |  |
| 23.711   | 4     | (3-parameter)       | 5.595220 | -1.60620 | 45.3653  | 0.287857 | ERR      |  |
| 19.209   | 4.5   |                     |          |          |          |          |          |  |
| 13.895   | 5     |                     |          |          |          |          |          |  |
| 11.804   | 5.5   |                     |          |          |          |          |          |  |
| 8.317    | 6     |                     |          |          |          |          |          |  |
| 4.337    | 6.5   |                     |          |          |          |          |          |  |
| 1.146    | 7     |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |

\* corresponds to data extracted from Table 26 on page 98.

# Regression of Batch-Reactor Biodegradation Data (with respect to time) : Variable Biomass

Data source -- Colish Thesis (data set #7)\*;

Substrate : o-chlorophenol

Culture : mlss

Condition : room temperature & pH 7.0-7.3

num.pts.= 15

| Raw Data |       |
|----------|-------|
| S(ppm)   | t(hr) |
| 39.665   | 0     |
| 36.011   | 0.5   |
| 37.724   | 1     |
| 37.165   | 1.5   |
| 39.422   | 2     |
| 34.92    | 2.5   |
| 29.626   | 3     |
| 27.539   | 3.5   |
| 23.711   | 4     |
| 19.209   | 4.5   |
| 13.895   | 5     |
| 11.804   | 5.5   |
| 8.317    | 6     |
| 4.337    | 6.5   |
| 1.146    | 7     |
| NA       | NA    |
| NA       | NA    |
| NA       | NA    |
| NA       | NA    |
| NA       | NA    |
| NA       | NA    |
| NA       | NA    |
| NA       | NA    |
| NA       | NA    |
| NA       | NA    |

## Summary of results:

| Kinetic Model  | ko       | K        | avg dt^2 | avg dS^2 |
|----------------|----------|----------|----------|----------|
| Zero-order     |          |          |          |          |
| (1-parameter)  | 0.006128 | ---      | 0.727958 | 17.92901 |
| First-order    |          |          |          |          |
| (1-parameter)  | 0.000407 | ---      | 3.455815 | 117.6294 |
| Monod Kinetics |          |          |          |          |
| (2-parameter)  | 0.004972 | -3.30753 | 0.613613 | ERR      |

Bo = 790 ppm \*\*  
Yc = 1.95 \*\*

\* corresponds to data extracted from Table 26 on page 98.

\*\* estimated from available MLSS measurements.

.....

Substrate : phenol  
Culture : m188  
Condition : 25C & neutral pH

Num.pts.= 7

[illegible]

E-20

\* simultaneous biodegradation with data set #1B extracted from Table 1 on page 21 of Mr. Prasad Gonnaphula thesis:

.....

Substrate : 2,6-dichlorophenol  
Culture : mlss  
Condition : 25C & neutral pH

Condition : 25C & neutral pH

E-21

\* simultaneous biodegradation with data set #1A from Table 1 on page 21 of Mr. Prasad Gonnaphula's thesis.

0000 0001 0010 0011 0100 0101 0110 0111 1000 1001 1010 1011 1100 1101 1110 1111 1200 1201 1210 1211 1220 1221 1230 1231 1240 1241 1250 1251 1260 1261 1270 1271 1280 1281 1290 1291 1300 1301 1310 1311 1320 1321 1330 1331 1340 1341 1350 1351 1360 1361 1370 1371 1380 1381 1390 1391 1400 1401 1410 1411 1420 1421 1430 1431 1440 1441 1450 1451 1460 1461 1470 1471 1480 1481 1490 1491 1500 1501 1510 1511 1520 1521 1530 1531 1540 1541 1550 1551 1560 1561 1570 1571 1580 1581 1590 1591 1600 1601 1610 1611 1620 1621 1630 1631 1640 1641 1650 1651 1660 1661 1670 1671 1680 1681 1690 1691 1700 1701 1710 1711 1720 1721 1730 1731 1740 1741 1750 1751 1760 1761 1770 1771 1780 1781 1790 1791 1800 1801 1810 1811 1820 1821 1830 1831 1840 1841 1850 1851 1860 1861 1870 1871 1880 1881 1890 1891 1900 1901 1910 1911 1920 1921 1930 1931 1940 1941 1950 1951 1960 1961 1970 1971 1980 1981 1990 1991 2000 2001 2010 2011 2020 2021 2030 2031 2040 2041 2050 2051 2060 2061 2070 2071 2080 2081 2090 2091 2100 2101 2110 2111 2120 2121 2130 2131 2140 2141 2150 2151 2160 2161 2170 2171 2180 2181 2190 2191 2200 2201 2210 2211 2220 2221 2230 2231 2240 2241 2250 2251 2260 2261 2270 2271 2280 2281 2290 2291 2300 2301 2310 2311 2320 2321 2330 2331 2340 2341 2350 2351 2360 2361 2370 2371 2380 2381 2390 2391 2400 2401 2410 2411 2420 2421 2430 2431 2440 2441 2450 2451 2460 2461 2470 2471 2480 2481 2490 2491 2500 2501 2510 2511 2520 2521 2530 2531 2540 2541 2550 2551 2560 2561 2570 2571 2580 2581 2590 2591 2600 2601 2610 2611 2620 2621 2630 2631 2640 2641 2650 2651 2660 2661 2670 2671 2680 2681 2690 2691 2700 2701 2710 2711 2720 2721 2730 2731 2740 2741 2750 2751 2760 2761 2770 2771 2780 2781 2790 2791 2800 2801 2810 2811 2820 2821 2830 2831 2840 2841 2850 2851 2860 2861 2870 2871 2880 2881 2890 2891 2900 2901 2910 2911 2920 2921 2930 2931 2940 2941 2950 2951 2960 2961 2970 2971 2980 2981 2990 2991 3000 3001 3010 3011 3020 3021 3030 3031 3040 3041 3050 3051 3060 3061 3070 3071 3080 3081 3090 3091 3100 3101 3110 3111 3120 3121 3130 3131 3140 3141 3150 3151 3160 3161 3170 3171 3180 3181 3190 3191 3200 3201 3210 3211 3220 3221 3230 3231 3240 3241 3250 3251 3260 3261 3270 3271 3280 3281 3290 3291 3300 3301 3310 3311 3320 3321 3330 3331 3340 3341 3350 3351 3360 3361 3370 3371 3380 3381 3390 3391 3400 3401 3410 3411 3420 3421 3430 3431 3440 3441 3450 3451 3460 3461 3470 3471 3480 3481 3490 3491 3500 3501 3510 3511 3520 3521 3530 3531 3540 3541 3550 3551 3560 3561 3570 3571 3580 3581 3590 3591 3600 3601 3610 3611 3620 3621 3630 3631 3640 3641 3650 3651 3660 3661 3670 3671 3680 3681 3690 3691 3700 3701 3710 3711 3720 3721 3730 3731 3740 3741 3750 3751 3760 3761 3770 3771 3780 3781 3790 3791 3800 3801 3810 3811 3820 3821 3830 3831 3840 3841 3850 3851 3860 3861 3870 3871 3880 3881 3890 3891 3900 3901 3910 3911 3920 3921 3930 3931 3940 3941 3950 3951 3960 3961 3970 3971 3980 3981 3990 3991 4000 4001 4010 4011 4020 4021 4030 4031 4040 4041 4050 4051 4060 4061 4070 4071 4080 4081 4090 4091 4100 4101 4110 4111 4120 4121 4130 4131 4140 4141 4150 4151 4160 4161 4170 4171 4180 4181 4190 4191 4200 4201 4210 4211 4220 4221 4230 4231 4240 4241 4250 4251 4260 4261 4270 4271 4280 4281 4290 4291 4300 4301 4310 4311 4320 4321 4330 4331 4340 4341 4350 4351 4360 4361 4370 4371 4380 4381 4390 4391 4400 4401 4410 4411 4420 4421 4430 4431 4440 4441 4450 4451 4460 4461 4470 4471 4480 4481 4490 4491 4500 4501 4510 4511 4520 4521 4530 4531 4540 4541 4550 4551 4560 4561 4570 4571 4580 4581 4590 4591 4600 4601 4610 4611 4620 4621 4630 4631 4640 4641 4650 4651 4660 4661 4670 4671 4680 4681 4690 4691 4700 4701 4710 4711 4720 4721 4730 4731 4740 4741 4750 4751 4760 4761 4770 4771 4780 4781 4790 4791 4800 4801 4810 4811 4820 4821 4830 4831 4840 4841 4850 4851 4860 4861 4870 4871 4880 4881 4890 4891 4900 4901 4910 4911 4920 4921 4930 4931 4940 4941 4950 4951 4960 4961 4970 4971 4980 4981 4990 4991 5000 5001 5010 5011 5020 5021 5030 5031 5040 5041 5050 5051 5060 5061 5070 5071 5080 5081 5090 5091 5100 5101 5110 5111 5120 5121 5130 5131 5140 5141 5150 5151 5160 5161 5170 5171 5180 5181 5190 5191 5200 5201 5210

Substrate : phenol  
Culture : m1ss  
Condition : 25C & neutral pH

Num.pts.= 7

[illegible]

E-22

\* simultaneous biodegradation with data set #2B extracted from Table 2 on page 22 of Mr. Prasad Gonnaphula' thesis.

1001 1002 1003 1004 1005 1006 1007 1008 1009 1010 1011 1012 1013 1014 1015 1016 1017 1018 1019 1020 1021 1022 1023 1024 1025 1026 1027 1028 1029 1030 1031 1032 1033 1034 1035 1036 1037 1038 1039 1040 1041 1042 1043 1044 1045 1046 1047 1048 1049 1050 1051 1052 1053 1054 1055 1056 1057 1058 1059 1060 1061 1062 1063 1064 1065 1066 1067 1068 1069 1070 1071 1072 1073 1074 1075 1076 1077 1078 1079 1080 1081 1082 1083 1084 1085 1086 1087 1088 1089 1090 1091 1092 1093 1094 1095 1096 1097 1098 1099 1100 1101 1102 1103 1104 1105 1106 1107 1108 1109 1110 1111 1112 1113 1114 1115 1116 1117 1118 1119 1120 1121 1122 1123 1124 1125 1126 1127 1128 1129 1130 1131 1132 1133 1134 1135 1136 1137 1138 1139 1140 1141 1142 1143 1144 1145 1146 1147 1148 1149 1150 1151 1152 1153 1154 1155 1156 1157 1158 1159 1160 1161 1162 1163 1164 1165 1166 1167 1168 1169 1170 1171 1172 1173 1174 1175 1176 1177 1178 1179 1180 1181 1182 1183 1184 1185 1186 1187 1188 1189 1190 1191 1192 1193 1194 1195 1196 1197 1198 1199 1200 1201 1202 1203 1204 1205 1206 1207 1208 1209 1210 1211 1212 1213 1214 1215 1216 1217 1218 1219 1220 1221 1222 1223 1224 1225 1226 1227 1228 1229 1230 1231 1232 1233 1234 1235 1236 1237 1238 1239 1240 1241 1242 1243 1244 1245 1246 1247 1248 1249 1250 1251 1252 1253 1254 1255 1256 1257 1258 1259 1260 1261 1262 1263 1264 1265 1266 1267 1268 1269 1270 1271 1272 1273 1274 1275 1276 1277 1278 1279 1280 1281 1282 1283 1284 1285 1286 1287 1288 1289 1290 1291 1292 1293 1294 1295 1296 1297 1298 1299 1300 1301 1302 1303 1304 1305 1306 1307 1308 1309 1310 1311 1312 1313 1314 1315 1316 1317 1318 1319 1320 1321 1322 1323 1324 1325 1326 1327 1328 1329 1330 1331 1332 1333 1334 1335 1336 1337 1338 1339 1340 1341 1342 1343 1344 1345 1346 1347 1348 1349 1350 1351 1352 1353 1354 1355 1356 1357 1358 1359 1360 1361 1362 1363 1364 1365 1366 1367 1368 1369 1370 1371 1372 1373 1374 1375 1376 1377 1378 1379 1380 1381 1382 1383 1384 1385 1386 1387 1388 1389 1390 1391 1392 1393 1394 1395 1396 1397 1398 1399 1400 1401 1402 1403 1404 1405 1406 1407 1408 1409 1410 1411 1412 1413 1414 1415 1416 1417 1418 1419 1420 1421 1422 1423 1424 1425 1426 1427 1428 1429 1430 1431 1432 1433 1434 1435 1436 1437 1438 1439 1440 1441 1442 1443 1444 1445 1446 1447 1448 1449 1450 1451 1452 1453 1454 1455 1456 1457 1458 1459 1460 1461 1462 1463 1464 1465 1466 1467 1468 1469 1470 1471 1472 1473 1474 1475 1476 1477 1478 1479 1480 1481 1482 1483 1484 1485 1486 1487 1488 1489 1490 1491 1492 1493 1494 1495 1496 1497 1498 1499 1500 1501 1502 1503 1504 1505 1506 1507 1508 1509 1510 1511 1512 1513 1514 1515 1516 1517 1518 1519 1520 1521 1522 1523 1524 1525 1526 1527 1528 1529 1530 1531 1532 1533 1534 1535 1536 1537 1538 1539 1540 1541 1542 1543 1544 1545 1546 1547 1548 1549 1550 1551 1552 1553 1554 1555 1556 1557 1558 1559 1560 1561 1562 1563 1564 1565 1566 1567 1568 1569 1570 1571 1572 1573 1574 1575 1576 1577 1578 1579 1580 1581 1582 1583 1584 1585 1586 1587 1588 1589 1590 1591 1592 1593 1594 1595 1596 1597 1598 1599 1600 1601 1602 1603 1604 1605 1606 1607 1608 1609 1610 1611 1612 1613 1614 1615 1616 1617 1618 1619 1620 1621 1622 1623 1624 1625 1626 1627 1628 1629 1630 1631 1632 1633 1634 1635 1636 1637 1638 1639 1640 1641 1642 1643 1644 1645 1646 1647 1648 1649 1650 1651 1652 1653 1654 1655 1656 1657 1658 1659 1660 1661 1662 1663 1664 1665 1666 1667 1668 1669 1670 1671 1672 1673 1674 1675 1676 1677 1678 1679 1680 1681 1682 1683 1684 1685 1686 1687 1688 1689 1690 1691 1692 1693 1694 1695 1696 1697 1698 1699 1700 1701 1702 1703 1704 1705 1706 1707 1708 1709 1710 1711 1712 1713 1714 1715 1716 1717 1718 1719 1720 1721 1722 1723 1724 1725 1726 1727 1728 1729 1730 1731 1732 1733 1734 1735 1736 1737 1738 1739 1740 1741 1742 1743 1744 1745 1746 1747 1748 1749 1750 1751 1752 1753 1754 1755 1756 1757 1758 1759 1760 1761 1762 1763 1764 1765 1766 1767 1768 1769 1770 1771 1772 1773 1774 1775 1776 1777 1778 1779 1780 1781 1782 1783 1784 1785 1786 1787 1788 1789 1790 1791 1792 1793 1794 1795 1796 1797 1798 1799 1800 1801 1802 1803 1804 1805 1806 1807 1808 1809 1810 1811 1812 1813 1814 1815 1816 1817 1818 1819

Substrate : 2,6-dichlorophenol  
Culture : m1ss  
Condition : 25C & neutral pH

um.pts.= 11

[illegible]

\* simultaneous biodegradation with data set #2A extracted from Table 2 on page 22 of Mr. Prasad Gonnaphula's thesis.



.....

um.pts.= 8

Substrate : phenol  
Culture : m1ss  
Condition : 25C & neutral pH

\_\_\_\_\_

[illegible]

E-24

\* simultaneous biodegradation with data set #3B extracted from Table 3 on page 23 of Mr. Prasad Gonnaphula's thesis.

.....

Data source -- Prasad Thesis (data set #3B) ;

Culture : miss

Condition : 25C & neutral pH

Num.pts.= 11

E-25

\* simultaneous biodegradation with data set #3A extracted from Table 3 on page 23 of Mr. Prasad Gonnaphula's thesis.

Substrate : phenol  
Culture : mlsa  
Condition : 25C & neutral pH

Substrate : phenol  
Culture : mlsa  
Condition : 25C & neutral pH

E-26

\* simultaneous biodegradation with data set #4B extracted from Table 4 on page 24 of Mr. Prasad Gonnaphula's thesis.

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Data source -- Prasad Thesis (data set #4B)<sup>^</sup>;

Culture : miss

Condition : 25C & neutral pH

Num.pts.= 4

E-27

\* simultaneous biodegradation with data set #4A extracted from Table 4 on page 24 of Mr. Prasad Gonnaphula's thesis.

-----

Substrate : phenol  
Culture : m1ss  
Condition : 21C & neutral pH

Num.pts.= 7

[illegible]

E-28

\* simultaneous biodegradation with data set #5B extracted from Table 5 of page 25 of Mr. Prasad Gonnaphula's thesis.

Substrate : 2,6-dichlorophenol  
Culture : mls  
Condition : 21C & neutral pH

Num.pts.= 7

[illegible]

\* simultaneous biodegradation with data set #5A extracted from Table 5 on page 25 of Mr. Prasad Gonnaphula's thesis.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Prasad Thesis (data set #6A)\*;

Substrate : phenol

Culture : mlss

Condition : 21C & neutral pH

Num.pts.= 12

| Raw Data |       | Summary of results: |  |          |          |          |          |          |
|----------|-------|---------------------|--|----------|----------|----------|----------|----------|
| S(ppm)   | t(hr) | Kinetic Model       |  | k        | K        | So       | avg dt^2 | avg dS^2 |
| 140.6    | 0     | Zero-order          |  |          |          |          |          |          |
| 142.5    | 0.42  | (1-parameter)       |  | 5.916785 | ---      | 140.6    | 7.602918 | 266.1656 |
| 128.5    | 1.42  | (2-parameter)       |  | 5.353486 | ---      | 130.7255 | 6.228442 | 178.5060 |
| 114.5    | 2.42  | First-order         |  |          |          |          |          |          |
| 112.5    | 3.42  | (1-parameter)       |  | 0.140308 | ---      | 140.6    | 8.443000 | 285.0632 |
| 100      | 4.42  | (2-parameter)       |  | 0.155950 | ---      | 197.8322 | 5.481822 | 588.2982 |
| 85.5     | 6.42  | Monod Kinetics      |  |          |          |          |          |          |
| 64       | 9.42  | (2-parameter)       |  | 11.08087 | 39.69368 | 140.6    | 1.326783 | 23.83599 |
| 41       | 11.42 | (3-parameter)       |  | 10.61288 | 37.12099 | 138.7603 | 1.310690 | 22.06392 |
| 9.7      | 23.58 |                     |  |          |          |          |          |          |
| 5.4      | 25.58 |                     |  |          |          |          |          |          |
| 1.2      | 27.91 |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |

\* simultaneous biodegradation with data set #6B extracted from Table 6 on page 26 of Mr. Prasad Gonnannhula's thesis.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Prasad Thesis (data set #6B)\*;

Substrate : 2-chlorophenol  
Culture : mlsa  
Condition : 21C & neutral pH

Num.pts.= 11

| Raw Data |       | Summary of results: |          |          |          |          |          |  |
|----------|-------|---------------------|----------|----------|----------|----------|----------|--|
| S(ppm)   | t(hr) | Kinetic Model       | k        | K        | So       | avg dt^2 | avg dS^2 |  |
| 13.6     | 0     | Zero-order          |          |          |          |          |          |  |
| 14.1     | 0.42  | (1-parameter)       | 0.442663 | ---      | 13.6     | 1.738072 | 0.340576 |  |
| 12.7     | 1.42  | (2-parameter)       | 0.457818 | ---      | 13.86600 | 1.548994 | 0.324665 |  |
| 12.1     | 2.42  | First-order         |          |          |          |          |          |  |
| 12       | 3.42  | (1-parameter)       | 0.067775 | ---      | 13.6     | 9.507647 | 2.927212 |  |
| 11.9     | 4.42  | (2-parameter)       | 0.077272 | ---      | 16.45877 | 5.341382 | 3.119672 |  |
| 10.5     | 6.42  | Monod Kinetics      |          |          |          |          |          |  |
| 10.2     | 9.42  | (2-parameter)       | 0.346385 | -1.49087 | 13.6     | 1.336737 | ERR      |  |
| 10       | 11.42 | (3-parameter)       | 0.353428 | -1.41253 | 13.6389  | 1.333352 | ERR      |  |
| 3        | 23.58 |                     |          |          |          |          |          |  |
| 1.9      | 25.58 |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |

E-31

\* simultaneous biodegradation with data set #6A extracted from Table 6 on page 26 of Mr. Prasad Gonnaphula's thesis.



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Num.pts.= 12

Substrate : phenol  
Culture : mlss  
Condition : 25C & neutral pH

E-32

\* simultaneous biodegradation with data set #7B extracted from Table 7 on page 27 of Mr. Prasad Gonnaphula's thesis.

.....

Num.pts.= 12

Substrate : 2-chlorophenol  
Culture : miss  
Condition : 25C & neutral pH

E-33

\* simultaneous biodegradation with data set #7A extracted from Table 7 on page 27 of Mr. Prasad Gonnaphūla's thesis.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Prasad Thesis (data set #8A)\* ;

Substrate : phenol  
Culture : mlss  
Condition : 25C & neutral pH

Num.pts.= 11

| Raw Data |       | Summary of results: |  |          |          |          |          |          |
|----------|-------|---------------------|--|----------|----------|----------|----------|----------|
| S(ppm)   | t(hr) | Kinetic Model       |  | k        | K        | So       | avg dt^2 | avg dS^2 |
| 95.5     | 0     | Zero-order          |  |          |          |          |          |          |
| 94.5     | 1     | (1-parameter)       |  | 8.176642 | ---      | 95.5     | 1.425481 | 95.30410 |
| 93       | 2     | (2-parameter)       |  | 9.825702 | ---      | 109.6011 | 0.529260 | 51.09712 |
| 83       | 3     | First-order         |  |          |          |          |          |          |
| 74.6     | 4     | (1-parameter)       |  | 0.266653 | ---      | 95.5     | 7.817324 | 807.2108 |
| 64.9     | 5     | (2-parameter)       |  | 0.384366 | ---      | 288.0366 | 2.842221 | 4678.628 |
| 52.61    | 7     | Monod Kinetics      |  |          |          |          |          |          |
| 37       | 8     | (2-parameter)       |  | 6.076627 | -8.99048 | 95.5     | 0.924666 | ERR      |
| 13.88    | 9     | (3-parameter)       |  | 7.858893 | -6.06117 | 105.4963 | 0.418316 | ERR      |
| 4.28     | 10    |                     |  |          |          |          |          |          |
| 2.8      | 11    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |

E-34

\* simultaneous biodegradation with data set #8B extracted from Table 8 on page 28 of Mr. Prasad Gonnaphula's thesis.

-----  
 Regresaion of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed  
 -----

Data source -- Prasad Thesis (data set #8B)\*;

Substrate : 2-chlorophenol  
 Culture : mlss  
 Condition : 25C & neutral pH

Num.pts.= 12

| Raw    | Data  | Summary of results: |               |          |          |          |          |          |
|--------|-------|---------------------|---------------|----------|----------|----------|----------|----------|
| S(ppm) | t(hr) | Kinetic             | Model         | k        | K        | So       | avg dt^2 | avg dS^2 |
| 10.75  | 0     | Zero-order          |               |          |          |          |          |          |
| 11.76  | 1     |                     | (1-parameter) | 0.614137 | ---      | 10.75    | 17.99957 | 6.788812 |
| 12.3   | 2     |                     | (2-parameter) | 0.915405 | ---      | 14.68159 | 3.145581 | 2.635894 |
| 12.25  | 3     | First-order         |               |          |          |          |          |          |
| 12     | 4     |                     | (1-parameter) | 0.086067 | ---      | 10.75    | 17.28262 | 9.189680 |
| 11.53  | 5     |                     | (2-parameter) | 0.130804 | ---      | 18.55404 | 3.836381 | 9.043135 |
| 10.57  | 7     | Monod Kinetics      |               |          |          |          |          |          |
| 8.85   | 8     |                     | (2-parameter) | -71.4453 | -837.089 | 10.75    | 17.28257 | 9.214332 |
| 7.39   | 9     |                     | (3-parameter) | 0.542382 | -2.97377 | 13.9236  | 3.003903 | ERR      |
| 5.26   | 10    |                     |               |          |          |          |          |          |
| 4.41   | 11    |                     |               |          |          |          |          |          |
| 3.2    | 12    |                     |               |          |          |          |          |          |
| NA     | NA    |                     |               |          |          |          |          |          |
| NA     | NA    |                     |               |          |          |          |          |          |
| NA     | NA    |                     |               |          |          |          |          |          |
| NA     | NA    |                     |               |          |          |          |          |          |
| NA     | NA    |                     |               |          |          |          |          |          |
| NA     | NA    |                     |               |          |          |          |          |          |
| NA     | NA    |                     |               |          |          |          |          |          |
| NA     | NA    |                     |               |          |          |          |          |          |
| NA     | NA    |                     |               |          |          |          |          |          |
| NA     | NA    |                     |               |          |          |          |          |          |
| NA     | NA    |                     |               |          |          |          |          |          |
| NA     | NA    |                     |               |          |          |          |          |          |
| NA     | NA    |                     |               |          |          |          |          |          |
| NA     | NA    |                     |               |          |          |          |          |          |
| NA     | NA    |                     |               |          |          |          |          |          |

135

\* simultaneous biodegradation with data set #8A extracted from Table 8 on page 28 of Mr. Prasad Gonnaphula's thesis.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Prasad Thesis (data set #9A)\*; Substrate : phenol  
Culture : mlsa  
Condition : 27C & neutral pH

Num.pts.= 12

| Raw Data |       | Summary of results: |          |          |          |          |          |
|----------|-------|---------------------|----------|----------|----------|----------|----------|
| S(ppm)   | t(hr) | Kinetic Model       | k        | K        | So       | avg dt^2 | avg dS^2 |
| 150      | 0     | Zero-order          |          |          |          |          |          |
| 140.2    | 1     | (1-parameter)       | 15.32631 | ---      | 150      | 0.309408 | 72.67871 |
| 114.3    | 2     | (2-parameter)       | 14.58328 | ---      | 144.4422 | 0.272827 | 58.02283 |
| 90.5     | 3     | First-order         |          |          |          |          |          |
| 80.3     | 4     | (1-parameter)       | 0.342623 | ---      | 150      | 4.395642 | 774.7662 |
| 67.5     | 5     | (2-parameter)       | 0.466073 | ---      | 436.9515 | 1.782996 | 8833.824 |
| 50.3     | 6     | Monod Kinetics      |          |          |          |          |          |
| 41       | 7     | (2-parameter)       | 18.73802 | 11.40344 | 150      | 0.054849 | 13.56828 |
| 22       | 8     | (3-parameter)       | 19.06536 | 11.93332 | 151.1734 | 0.053951 | 13.62580 |
| 10.31    | 9     |                     |          |          |          |          |          |
| 3.2      | 10    |                     |          |          |          |          |          |
| 1.2      | 11    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |

\* simultaneous biodegradation with data set #9B extracted from Table 9 on page 29 of Mr. Prasad Gonnaphula's thesis.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Prasad Thesis (data set #9B)\*;

Substrate : 2-chlorophenol

Culture : mlsa

Condition : 27C & neutral pH

Num.pts.= 11

| Raw Data |       | Summary of results: |          |          |          |          |          |  |
|----------|-------|---------------------|----------|----------|----------|----------|----------|--|
| S(ppm)   | t(hr) | Kinetic Model       | k        | K        | So       | avg dt^2 | avg dS^2 |  |
| 21.93    | 0     | Zero-order          |          |          |          |          |          |  |
| 22.15    | 1     | (1-parameter)       | 2.097752 | ---      | 21.93    | 0.290129 | 1.276733 |  |
| 19.58    | 2     | (2-parameter)       | 2.329542 | ---      | 23.62589 | 0.103790 | 0.563245 |  |
| 17.3     | 3     | First-order         |          |          |          |          |          |  |
| 14.7     | 4     | (1-parameter)       | 0.236036 | ---      | 21.93    | 3.598483 | 17.17133 |  |
| 11.6     | 5     | (2-parameter)       | 0.320723 | ---      | 43.22241 | 1.312364 | 52.96274 |  |
| 8.9      | 6     | Monod Kinetics      |          |          |          |          |          |  |
| 7.3      | 7     | (2-parameter)       | 1.966904 | -0.60901 | 21.93    | 0.276014 | ERR      |  |
| 5.1      | 8     | (3-parameter)       | 2.458725 | 0.462633 | 23.8062  | 0.099470 | 0.551961 |  |
| 2.1      | 9     |                     |          |          |          |          |          |  |
| 1.1      | 10    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |

E-37

\* simultaneous biodegradation with data set #9A extracted from Table 9 on page 29 of Mr. Prasad Gonnaphula's thesis.

---

Culture : miss

Condition : 27C & neutral pH

E-38

\* simultaneous biodegradation with data set #10B extracted from Table 10 on page 30 of Mr. Prasad Gonnaphula's thesis.

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Substrate : 2-chlorophenol  
Culture : m1ss  
Condition : 27C & neutral pH

Num.pts.= 7

[illegible]

7-39

\* simultaneous biodegradation with data set #10A extracted from Table 10 on page 30 of Mr. Prasad Gonnaphula's thesis.



Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Prasad Thesis (data set #11A)\*;

Substrate : phenol  
Culture : m1ss  
Condition : 31C & neutral pH

Num.pts.= 14

| Raw    | Data  | Summary of results: |          |          |          |          |          |
|--------|-------|---------------------|----------|----------|----------|----------|----------|
| S(ppm) | t(hr) | Kinetic Model       | k        | K        | So       | avg dt^2 | avg dS^2 |
| 122.5  | 0     | Zero-order          |          |          |          |          |          |
| 127.9  | 1     | (1-parameter)       | 4.271858 | ---      | 122.5    | 3.845950 | 70.18389 |
| 127.33 | 2     | (2-parameter)       | 4.563115 | ---      | 129.8467 | 2.686988 | 55.94853 |
| 121.66 | 3     | First-order         |          |          |          |          |          |
| 118.02 | 4     | (1-parameter)       | 0.132265 | ---      | 122.5    | 33.86905 | 621.5093 |
| 105.5  | 5     | (2-parameter)       | 0.161255 | ---      | 266.3904 | 21.05997 | 2748.237 |
| 80.5   | 6.25  | Monod Kinetics      |          |          |          |          |          |
| 29.9   | 22.75 | (2-parameter)       | 4.495504 | 1.858292 | 122.5    | 3.754767 | 68.07259 |
| 22.5   | 23.75 | (3-parameter)       | 5.055253 | 3.589436 | 131.1224 | 2.427145 | 50.25916 |
| 16.5   | 25    |                     |          |          |          |          |          |
| 3.5    | 26.16 |                     |          |          |          |          |          |
| 2.5    | 27.32 |                     |          |          |          |          |          |
| 1.6    | 28.8  |                     |          |          |          |          |          |
| 1      | 30.3  |                     |          |          |          |          |          |
| NA     | NA    |                     |          |          |          |          |          |
| NA     | NA    |                     |          |          |          |          |          |
| NA     | NA    |                     |          |          |          |          |          |
| NA     | NA    |                     |          |          |          |          |          |
| NA     | NA    |                     |          |          |          |          |          |
| NA     | NA    |                     |          |          |          |          |          |
| NA     | NA    |                     |          |          |          |          |          |
| NA     | NA    |                     |          |          |          |          |          |
| NA     | NA    |                     |          |          |          |          |          |
| NA     | NA    |                     |          |          |          |          |          |
| NA     | NA    |                     |          |          |          |          |          |
| NA     | NA    |                     |          |          |          |          |          |

E-40

\* simultaneous biodegradation with data set #11B extracted from Table 11 on page 31 of Mr. Prasad Gonnaphula's thesis.

# Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Prasad Thesis (data set #11B)\*;

Substrate : nitrobenzene

Culture : mlss

Condition : 31C & neutral pH

Num.pts.= 15

| Raw Data |       | Summary of results: |  |          |          |          |          |          |
|----------|-------|---------------------|--|----------|----------|----------|----------|----------|
| S(ppm)   | t(hr) | Kinetic Model       |  | k        | K        | So       | avg dt^2 | avg dS^2 |
| 19       | 0     | Zero-order          |  |          |          |          |          |          |
| 19       | 1     | (1-parameter)       |  | 0.538576 | ---      | 19       | 10.07260 | 2.921702 |
| 19.9     | 2     | (2-parameter)       |  | 0.607473 | ---      | 20.85490 | 5.707882 | 2.106347 |
| 19.78    | 3     | First-order         |  |          |          |          |          |          |
| 18.65    | 4     | (1-parameter)       |  | 0.075982 | ---      | 19       | 61.21094 | 13.63091 |
| 17.07    | 5     | (2-parameter)       |  | 0.099600 | ---      | 36.82137 | 35.88558 | 57.43534 |
| 16.2     | 6.25  | Monod Kinetics      |  |          |          |          |          |          |
| 9.23     | 22.75 | (2-parameter)       |  | 0.381919 | -2.29983 | 19       | 4.933967 | 2.476828 |
| 8.8      | 23.75 | (3-parameter)       |  | 0.432099 | -2.11409 | 20.1328  | 2.555188 | ERR      |
| 8.3      | 25    |                     |  |          |          |          |          |          |
| 5.8      | 26.16 |                     |  |          |          |          |          |          |
| 4        | 27.32 |                     |  |          |          |          |          |          |
| 1.5      | 28.8  |                     |  |          |          |          |          |          |
| 1.08     | 30.3  |                     |  |          |          |          |          |          |
| 1.01     | 30.9  |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |

\*simultaneous biodegradation with data set #11A extracted from Table 11 on page 31 of Mr. Prasad Gonnaphula's thesis.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Prasad Thesis (data set #12A) \*;

Substrate : phenol  
Culture : mlsa  
Condition : 31C & neutral pH

Num.pts.= 14

| Raw    | Data  | Summary of results: |       |          |          |          |                   |
|--------|-------|---------------------|-------|----------|----------|----------|-------------------|
| S(ppm) | t(hr) | Kinetic             | Model | k        | K        | So       | avg dt^2 avg dS^2 |
| 101.5  | 0     | Zero-order          |       |          |          |          |                   |
| 112.5  | 1     | (1-parameter)       |       | 3.563000 | ---      | 101.5    | 11.19786 142.1566 |
| 118    | 2     | (2-parameter)       |       | 4.074454 | ---      | 115.0879 | 5.497992 91.27315 |
| 112.24 | 3     | First-order         |       |          |          |          |                   |
| 101.6  | 4     | (1-parameter)       |       | 0.119906 | ---      | 101.5    | 30.67667 548.5982 |
| 95.5   | 5     | (2-parameter)       |       | 0.145767 | ---      | 204.5701 | 17.77639 1253.750 |
| 63     | 6.25  | Monod Kinetics      |       |          |          |          |                   |
| 28.5   | 22.75 | (2-parameter)       |       | 4.253354 | 6.193876 | 101.5    | 10.36531 155.6258 |
| 17.9   | 23.75 | (3-parameter)       |       | 5.058611 | 7.684290 | 117.3658 | 4.592302 88.66798 |
| 13.4   | 25    |                     |       |          |          |          |                   |
| 4.12   | 26.15 |                     |       |          |          |          |                   |
| 3      | 27.35 |                     |       |          |          |          |                   |
| 2.54   | 28.8  |                     |       |          |          |          |                   |
| 1.15   | 30.2  |                     |       |          |          |          |                   |
| NA     | NA    |                     |       |          |          |          |                   |
| NA     | NA    |                     |       |          |          |          |                   |
| NA     | NA    |                     |       |          |          |          |                   |
| NA     | NA    |                     |       |          |          |          |                   |
| NA     | NA    |                     |       |          |          |          |                   |
| NA     | NA    |                     |       |          |          |          |                   |
| NA     | NA    |                     |       |          |          |          |                   |
| NA     | NA    |                     |       |          |          |          |                   |
| NA     | NA    |                     |       |          |          |          |                   |
| NA     | NA    |                     |       |          |          |          |                   |
| NA     | NA    |                     |       |          |          |          |                   |
| NA     | NA    |                     |       |          |          |          |                   |

E-42

\* simultaneous biodegradation with data set #12B extracted from Table 12 on page 32 of Mr. Prasad Gonnaphula's thesis.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Prasad Thesis (data set #12B)\*;

Substrate : nitrobenzene  
Culture : mlsa  
Condition : 31C & neutral pH

Num.pts.= 14

| Raw Data |       | Summary of results: |          |          |          |          |          |     |
|----------|-------|---------------------|----------|----------|----------|----------|----------|-----|
| S(ppm)   | t(hr) | Kinetic Model       | k        | K        | So       | avg dt^2 | avg dS^2 |     |
| 19.58    | 0     | Zero-order          |          |          |          |          |          |     |
| 19.6     | 1     | (1-parameter)       | 0.558738 | ---      | 19.58    | 6.127315 | 1.912880 |     |
| 21.1     | 2     | (2-parameter)       | 0.622448 | ---      | 21.24625 | 2.619198 | 1.014788 |     |
| 20.9     | 3     | First-order         |          |          |          |          |          |     |
| 18.5     | 4     | (1-parameter)       | 0.061633 | ---      | 19.58    | 27.62255 | 7.229949 |     |
| 17.9     | 5     | (2-parameter)       | 0.074046 | ---      | 27.32247 | 16.58279 | 9.485779 |     |
| 16.5     | 6.25  | Monod Kinetics      |          |          |          |          |          |     |
| 8.3      | 22.75 | (2-parameter)       | 0.438265 | -2.05916 | 19.58    | 5.033616 |          | ERR |
| 7        | 23.75 | (3-parameter)       | 0.509970 | -1.66209 | 20.9611  | 2.110781 |          | ERR |
| 6.8      | 25    |                     |          |          |          |          |          |     |
| 5.9      | 26.15 |                     |          |          |          |          |          |     |
| 3.4      | 27.35 |                     |          |          |          |          |          |     |
| 2.19     | 28.8  |                     |          |          |          |          |          |     |
| 2.02     | 30.2  |                     |          |          |          |          |          |     |
| NA       | NA    |                     |          |          |          |          |          |     |
| NA       | NA    |                     |          |          |          |          |          |     |
| NA       | NA    |                     |          |          |          |          |          |     |
| NA       | NA    |                     |          |          |          |          |          |     |
| NA       | NA    |                     |          |          |          |          |          |     |
| NA       | NA    |                     |          |          |          |          |          |     |
| NA       | NA    |                     |          |          |          |          |          |     |
| NA       | NA    |                     |          |          |          |          |          |     |
| NA       | NA    |                     |          |          |          |          |          |     |
| NA       | NA    |                     |          |          |          |          |          |     |
| NA       | NA    |                     |          |          |          |          |          |     |

E-43

\* simultaneous biodegradation with data set #12A extracted from Table 12 on page 32 of Mr. Prasad Gonnaphula's thesis.

---

Substrate : phenol  
Culture : m1ss  
Condition : 22C & neutral pH

Num.pts.= 7

[illegible]

E-44

\* simultaneous biodegradation with data set #13B extracted from Table 13 on page 33 of Mr. Prasad Gonnaphula's thesis.

.....

Substrate : nitrobenzene  
Culture : m1ss  
Condition : 22C & neutral pH

Num.pts.= 7

[illegible]

E-45

\* simultaneous biodegradation with data set #13A extracted from Table 13 on page 33 of Mr. Prasad Gonnaphula's thesis.

-----

Substrate : phenol  
Culture : mlss  
Condition : 22C & neutral pH

Num.pts.= 7

[illegible]

E-46

\* simultaneous biodegradation with data set #14B extracted from Table 14 on page 34 of Mr. Prasad Gonnaphula's thesis.

Substrate : nitrobenzene  
Culture : mlss  
Condition : 22C & neutral pH

Num.pts.= 7

[illegible]

E-47

\* simultaneous biodegradation with data set #14A extracted from Table 14 on page 34 of Mr. Prasad Gonnaphula's thesis.



.....

Substrate : phenol  
Culture : m1ss  
Condition : 27C & pH 6.2-6.3

Num.pts.= 6

[illegible]

\* corresponds to data extracted from Table 8 on page 63.

\*\*units are ppm/min for zero-order & Monod and 1/min for first-order.

Substrate : phenol  
Culture : m155  
Condition : 27C & pH 6.2-6.3

6

Summary of results:

Bo = 382 ppm \*\*\*  
Yc = -0.617 \*\*\*

\*\*\*estimated from available MLSS measurements.

---

Substrate : phenol  
Culture : mls  
Condition : 27C & pH 6.0-6.3

Num.pts.= 7

[illegible]

\*\*units are ppm/min for zero-order & Monod and 1/min for first-order.

---

Substrate : phenol  
Culture : m1aa  
Condition : 27C & pH 6.0-6.3

Substrate : phenol  
Culture : m1aa  
Condition : 27C & pH 6.0-6.3

E-51

\* corresponds to data extracted from Table 9 on page 64.  
 \*\* units are ppm/ppm-min for zero-order & Monod and 1/ppm-min for first-order.  
 \*\*\*estimated from available MLSS measurements.

.....

Substrate : o-chlorophenol  
Culture : m155  
Condition : 27C & pH 7.2

Num.pts.= 9

[illegible]

\* corresponds to data extracted from Table 30 on page 85.

```
**units are ppm/min for zero-order & Monod and 1/min for first-order.
```

.....

Substrate : o-chlorophenol  
Culture : mlssa  
Condition : 27C & pH 7.2

Num.pts.= 9

[illegible]

Bo = 374 ppm\*\*\*  
Yc = -3.214\*\*\*

\* corresponds to data extracted from Table 30 on page 85.

\*\* units are ppm/ppm-min for zero-order & Monod and 1/ppm-min for first-order.

\*\*\*estimated from available MLSS measurements.

1000 1001 1002 1003 1004 1005 1006 1007 1008 1009 1010 1011 1012 1013 1014 1015 1016 1017 1018 1019 1020 1021 1022 1023 1024 1025 1026 1027 1028 1029 1030 1031 1032 1033 1034 1035 1036 1037 1038 1039 1040 1041 1042 1043 1044 1045 1046 1047 1048 1049 1050 1051 1052 1053 1054 1055 1056 1057 1058 1059 1060 1061 1062 1063 1064 1065 1066 1067 1068 1069 1070 1071 1072 1073 1074 1075 1076 1077 1078 1079 1080 1081 1082 1083 1084 1085 1086 1087 1088 1089 1090 1091 1092 1093 1094 1095 1096 1097 1098 1099 1100 1101 1102 1103 1104 1105 1106 1107 1108 1109 1110 1111 1112 1113 1114 1115 1116 1117 1118 1119 1120 1121 1122 1123 1124 1125 1126 1127 1128 1129 1130 1131 1132 1133 1134 1135 1136 1137 1138 1139 1140 1141 1142 1143 1144 1145 1146 1147 1148 1149 1150 1151 1152 1153 1154 1155 1156 1157 1158 1159 1160 1161 1162 1163 1164 1165 1166 1167 1168 1169 1170 1171 1172 1173 1174 1175 1176 1177 1178 1179 1180 1181 1182 1183 1184 1185 1186 1187 1188 1189 1190 1191 1192 1193 1194 1195 1196 1197 1198 1199 1200 1201 1202 1203 1204 1205 1206 1207 1208 1209 1210 1211 1212 1213 1214 1215 1216 1217 1218 1219 1220 1221 1222 1223 1224 1225 1226 1227 1228 1229 1230 1231 1232 1233 1234 1235 1236 1237 1238 1239 1240 1241 1242 1243 1244 1245 1246 1247 1248 1249 1250 1251 1252 1253 1254 1255 1256 1257 1258 1259 1260 1261 1262 1263 1264 1265 1266 1267 1268 1269 1270 1271 1272 1273 1274 1275 1276 1277 1278 1279 1280 1281 1282 1283 1284 1285 1286 1287 1288 1289 1290 1291 1292 1293 1294 1295 1296 1297 1298 1299 1300 1301 1302 1303 1304 1305 1306 1307 1308 1309 1310 1311 1312 1313 1314 1315 1316 1317 1318 1319 1320 1321 1322 1323 1324 1325 1326 1327 1328 1329 1330 1331 1332 1333 1334 1335 1336 1337 1338 1339 1340 1341 1342 1343 1344 1345 1346 1347 1348 1349 1350 1351 1352 1353 1354 1355 1356 1357 1358 1359 1360 1361 1362 1363 1364 1365 1366 1367 1368 1369 1370 1371 1372 1373 1374 1375 1376 1377 1378 1379 1380 1381 1382 1383 1384 1385 1386 1387 1388 1389 1390 1391 1392 1393 1394 1395 1396 1397 1398 1399 1400 1401 1402 1403 1404 1405 1406 1407 1408 1409 1410 1411 1412 1413 1414 1415 1416 1417 1418 1419 1420 1421 1422 1423 1424 1425 1426 1427 1428 1429 1430 1431 1432 1433 1434 1435 1436 1437 1438 1439 1440 1441 1442 1443 1444 1445 1446 1447 1448 1449 1450 1451 1452 1453 1454 1455 1456 1457 1458 1459 1460 1461 1462 1463 1464 1465 1466 1467 1468 1469 1470 1471 1472 1473 1474 1475 1476 1477 1478 1479 1480 1481 1482 1483 1484 1485 1486 1487 1488 1489 1490 1491 1492 1493 1494 1495 1496 1497 1498 1499 1500 1501 1502 1503 1504 1505 1506 1507 1508 1509 1510 1511 1512 1513 1514 1515 1516 1517 1518 1519 1520 1521 1522 1523 1524 1525 1526 1527 1528 1529 1530 1531 1532 1533 1534 1535 1536 1537 1538 1539 1540 1541 1542 1543 1544 1545 1546 1547 1548 1549 1550 1551 1552 1553 1554 1555 1556 1557 1558 1559 1560 1561 1562 1563 1564 1565 1566 1567 1568 1569 1570 1571 1572 1573 1574 1575 1576 1577 1578 1579 1580 1581 1582 1583 1584 1585 1586 1587 1588 1589 1590 1591 1592 1593 1594 1595 1596 1597 1598 1599 1600 1601 1602 1603 1604 1605 1606 1607 1608 1609 1610 1611 1612 1613 1614 1615 1616 1617 1618 1619 1620 1621 1622 1623 1624 1625 1626 1627 1628 1629 1630 1631 1632 1633 1634 1635 1636 1637 1638 1639 1640 1641 1642 1643 1644 1645 1646 1647 1648 1649 1650 1651 1652 1653 1654 1655 1656 1657 1658 1659 1660 1661 1662 1663 1664 1665 1666 1667 1668 1669 1670 1671 1672 1673 1674 1675 1676 1677 1678 1679 1680 1681 1682 1683 1684 1685 1686 1687 1688 1689 1690 1691 1692 1693 1694 1695 1696 1697 1698 1699 1700 1701 1702 1703 1704 1705 1706 1707 1708 1709 1710 1711 1712 1713 1714 1715 1716 1717 1718 1719 1720 1721 1722 1723 1724 1725 1726 1727 1728 1729 1730 1731 1732 1733 1734 1735 1736 1737 1738 1739 1740 1741 1742 1743 1744 1745 1746 1747 1748 1749 1750 1751 1752 1753 1754 1755 1756 1757 1758 1759 1760 1761 1762 1763 1764 1765 1766 1767 1768 1769 1770 1771 1772 1773 1774 1775 1776 1777 1778 1779 1780 1781 1782 1783 1784 1785 1786 1787 1788 1789 1790 1791 1792 1793 1794 1795 1796 1797 1798 1799 1800 1801 1802 1803 1804 1805 1806 1807 1808 1809 1810 1811 1812 1813 1814 1815 1816 1817 1

Condition : 27C & pH 6.7

Num.pts.= 7

E-54

\*\*units are ppm/min for zero-order and Monod and 1/min for first-order.

.....

Substrate : o-chlorophenol  
Culture : mls  
Condition : 27C & pH 6.7

Num.pts.= 7

[illegible]

Bo = 363 ppm \*\*\*  
Yc = -5.172 \*\*\*

\* corresponds to data extracted from Table 31 on page 86.

\*\* units are ppm/ppm-min for zero-order & Monod and 1/ppm-min for first-order.

\*\*\*estimated from available MLSS measurements.



---

Substrate : o-chlorophenol  
Culture : miss  
Condition : 28C & pH 6.6-6.7

Substrate : o-chlorophenol  
Culture : miss  
Condition : 28C & pH 6.6-6.7

E-56

\*\*units are ppm/min for zero-order & Monod and 1/min for first-order.

.....

Culture : miss

Condition : 28C & pH 6.6.-6.7

Num.pts.= 7

[illegible]
$$Y_C = -0.106***$$

\* corresponds to data extracted from Table 32 on page 87.

\*\* units are ppm/ppm-min for zero-order & Monod and 1/ppm-min for first-order.

\*\*\*estimated from available MLSS measurements.

-----

Substrate : phenol  
Culture : unacclimated sludge  
Condition : 25C & neutral pH

Num.pts.= 6

[illegible]

7158

\* simultaneous biodegradation with data sets #1B & #1C extracted from Table 3.

[illegible]

Substrate : nitrobenzene  
Culture : unacclimated sludge  
Condition : 25C & neutral pH

E-59

\* simultaneous biodegradation with data sets #1A & #1C extracted from Table 3.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Naik Thesis (data set #1C)\*; Substrate : 2,6-dichlorophenol  
Culture : unacclimated sludge  
Condition : 25C & neutral pH

Num.pts.= 18

| Raw Data |       | Summary of results: |  |          |          |          |          |          |
|----------|-------|---------------------|--|----------|----------|----------|----------|----------|
| S(ppm)   | t(hr) | Kinetic Model       |  | k        | K        | So       | avg dt^2 | avg dS^2 |
| 8.1      | 0     | Zero-order          |  |          |          |          |          |          |
| 7.7      | 1     | (1-parameter)       |  | 0.041488 | ---      | 8.1      | 1029.806 | 1.772592 |
| 7.9      | 2     | (2-parameter)       |  | 0.059381 | ---      | 9.494008 | 666.2502 | 2.349279 |
| 7.8      | 3     | First-order         |  |          |          |          |          |          |
| 7        | 5     | (1-parameter)       |  | 0.008122 | ---      | 8.1      | 1250.506 | 2.778653 |
| 7.7      | 7     | (2-parameter)       |  | 0.012065 | ---      | 11.20923 | 722.5130 | 5.421691 |
| 7.5      | 19    | Monod Kinetics      |  |          |          |          |          |          |
| 7.9      | 22    | (2-parameter)       |  | 0.011439 | -3.94896 | 8.1      | 777.0406 | 1.036612 |
| 7.6      | 26    | (3-parameter)       |  | 0.019812 | -3.45746 | 8.7133   | 619.8855 | 1.119745 |
| 7.8      | 42    |                     |  |          |          |          |          |          |
| 7.9      | 48    |                     |  |          |          |          |          |          |
| 8        | 54    |                     |  |          |          |          |          |          |
| 7.5      | 67    |                     |  |          |          |          |          |          |
| 7.7      | 77    |                     |  |          |          |          |          |          |
| 6.6      | 91    |                     |  |          |          |          |          |          |
| 4.8      | 96    |                     |  |          |          |          |          |          |
| 3.9      | 97    |                     |  |          |          |          |          |          |
| 2.6      | 99    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |

\* simultaneous biodegradation with data sets #1A & #1B extracted from Table 3.

-----

Substrate : phenol  
Culture : unacclimated sludge  
Condition : 25C & neutral pH

lum.pts.= 6

[illegible]

E-61

\* simultaneous biodegradation with data sets #2B & #2C extracted from Table 4 on page 22.

.....

```
data source -- Naik Thesis (data set #2B)^;
```

Substrate : nitrobenzene  
Culture : unacclimated sludge  
Condition : 25C & neutral pH

um.pts.= 6

[illegible]

E-62

\* simultaneous biodegradation with data sets #2A & #2C extracted from Table 4 on page 22.

---

Substrate : 2,6-dichlorophenol  
Culture : unacclimated sludge  
Condition : 25C & neutral pH

[illegible]

\_\_\_\_\_

E-63

\* simultaneous biodegradation with data sets #2A & #2B extracted from Table 4 on page 22.



.....

Culture : unacclimated sludge  
Condition : 25C & neutral pH

E-64

\* simultaneous biodegradation with data sets #3B & #3C extracted from Table 5.

.....

Substrate : nitrobenzene  
Culture : unacclimated sludge  
Condition : 25C & neutral pH

Num.pts.= 6

[illegible]

E-65

\* simultaneous biodegradation with data sets #3A & #3C extracted from Table 5.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Naik Thesis (data set #3C)\*;

Substrate : 2,6-dichlorophenol  
Culture : unacclimated sludge  
Condition : 25C & neutral pH

Num.pts.= 18

| Raw Data |       | Summary of results: |          |          |          |                     |                     |
|----------|-------|---------------------|----------|----------|----------|---------------------|---------------------|
| S(ppm)   | t(hr) | Kinetic Model       | k        | K        | So       | avg dt <sup>2</sup> | avg dS <sup>2</sup> |
| 8.7      | 0     | Zero-order          |          |          |          |                     |                     |
| 7.9      | 1     | (1-parameter)       | 0.048274 | ---      | 8.7      | 760.8869            | 1.773204            |
| 7.9      | 2     | (2-parameter)       | 0.063723 | ---      | 9.815264 | 591.7872            | 2.403040            |
| 8.2      | 3     | First-order         |          |          |          |                     |                     |
| 7.8      | 5     | (1-parameter)       | 0.009346 | ---      | 8.7      | 1053.149            | 3.045663            |
| 7.7      | 7     | (2-parameter)       | 0.013450 | ---      | 11.98627 | 675.7426            | 6.573213            |
| 7.9      | 19    | Monod Kinetics      |          |          |          |                     |                     |
| 7.8      | 22    | (2-parameter)       | 0.016130 | -3.72522 | 8.7      | 516.8474            | 1.177402            |
| 8.1      | 26    | (3-parameter)       | 0.019033 | -3.56531 | 8.8849   | 507.1387            | 1.157618            |
| 8        | 42    |                     |          |          |          |                     |                     |
| 7.9      | 48    |                     |          |          |          |                     |                     |
| 8.1      | 54    |                     |          |          |          |                     |                     |
| 7.9      | 67    |                     |          |          |          |                     |                     |
| 7.7      | 77    |                     |          |          |          |                     |                     |
| 6.5      | 91    |                     |          |          |          |                     |                     |
| 4.6      | 96    |                     |          |          |          |                     |                     |
| 3.5      | 97    |                     |          |          |          |                     |                     |
| 2.3      | 99    |                     |          |          |          |                     |                     |
| NA       | NA    |                     |          |          |          |                     |                     |
| NA       | NA    |                     |          |          |          |                     |                     |
| NA       | NA    |                     |          |          |          |                     |                     |
| NA       | NA    |                     |          |          |          |                     |                     |
| NA       | NA    |                     |          |          |          |                     |                     |
| NA       | NA    |                     |          |          |          |                     |                     |
| NA       | NA    |                     |          |          |          |                     |                     |

E-66

\* simultaneous biodegradation with data sets #3A & #3B extracted from Table 5.

```
Data source -- Naik Thesis (data set #4A) ;
```

Substrate : phenol  
Culture : unacclimated sludge  
Condition : 25C & neutral pH

Num.pts.= 6

[illegible]

E-67

\* simultaneous biodegradation with data sets #4B & #4C extracted from Table 6.

---

Substrate : nitrobenzene  
Culture : unacclimated sludge  
Condition : 25C & neutral pH

Substrate : nitrobenzene  
Culture : unacclimated sludge  
Condition : 25C & neutral pH

E-68

\* simultaneous biodegradation with data sets #4A & #4C extracted from Table 6.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Naik Thesis (data set #4C) \*

Substrate : 2,6-dichlorophenol  
Culture : unacclimated aludge  
Condition : 25C & neutral pH

Num.pts.= 13

| Raw Data |       | Summary of results: |          |          |          |                     |                     |  |
|----------|-------|---------------------|----------|----------|----------|---------------------|---------------------|--|
| S(ppm)   | t(hr) | Kinetic Model       | k        | K        | So       | avg dt <sup>2</sup> | avg dS <sup>2</sup> |  |
| 7.9      | 0     | Zero-order          |          |          |          |                     |                     |  |
| 8        | 1     | (1-parameter)       | 0.165958 | ---      | 7.9      | 68.14675            | 1.876919            |  |
| 8.1      | 2     | (2-parameter)       | 0.236568 | ---      | 9.639164 | 33.93281            | 1.899033            |  |
| 7.9      | 3     | First-order         |          |          |          |                     |                     |  |
| 7.8      | 5     | (1-parameter)       | 0.034971 | ---      | 7.9      | 93.66637            | 2.996199            |  |
| 8        | 7     | (2-parameter)       | 0.053071 | ---      | 12.37092 | 45.17932            | 6.160307            |  |
| 7.9      | 19    | Monod Kinetics      |          |          |          |                     |                     |  |
| 6.6      | 21    | (2-parameter)       | 0.055333 | -3.40183 | 7.9      | 46.84371            | 1.281584            |  |
| 6        | 22    | (3-parameter)       | 0.076231 | -3.35475 | 8.7011   | 23.77503            | 1.129769            |  |
| 5.3      | 23    |                     |          |          |          |                     |                     |  |
| 4.2      | 24    |                     |          |          |          |                     |                     |  |
| 3.4      | 25    |                     |          |          |          |                     |                     |  |
| 2.1      | 26    |                     |          |          |          |                     |                     |  |
| NA       | NA    |                     |          |          |          |                     |                     |  |
| NA       | NA    |                     |          |          |          |                     |                     |  |
| NA       | NA    |                     |          |          |          |                     |                     |  |
| NA       | NA    |                     |          |          |          |                     |                     |  |
| NA       | NA    |                     |          |          |          |                     |                     |  |
| NA       | NA    |                     |          |          |          |                     |                     |  |
| NA       | NA    |                     |          |          |          |                     |                     |  |
| NA       | NA    |                     |          |          |          |                     |                     |  |
| NA       | NA    |                     |          |          |          |                     |                     |  |
| NA       | NA    |                     |          |          |          |                     |                     |  |
| NA       | NA    |                     |          |          |          |                     |                     |  |
| NA       | NA    |                     |          |          |          |                     |                     |  |
| NA       | NA    |                     |          |          |          |                     |                     |  |

E-69

\* simultaneous biodegradation with data sets #4A & #4B extracted from Table 6.

Data source -- Naik Thesis (data set #5A)\*;

Substrate : phenol  
Culture : phenol-acclimated sludge  
Condition : 25C & neutral pH

Num.pts.= 5

[illegible]

E-70

\* simultaneous biodegradation with data sets #5B & #5C extracted from Table 7.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Conatant Biomass Assumed

Data source -- Naik Thesis (data set #5B)\*;

Substrate : nitrobenzene  
Culture : phenol-acclimated sludge  
Condition : 25C & neutral pH

Num.pts.= 12

| Raw Data |       | Summary of results: |  |          |          |          |          |          |
|----------|-------|---------------------|--|----------|----------|----------|----------|----------|
| S(ppm)   | t(hr) | Kinetic Model       |  | k        | K        | So       | avg dt^2 | avg dS^2 |
| 10       | 0     | Zero-order          |  |          |          |          |          |          |
| 9.4      | 0.5   | (1-parameter)       |  | 0.824363 | ---      | 10       | 0.842410 | 0.572481 |
| 9.6      | 1     | (2-parameter)       |  | 0.988146 | ---      | 10.95999 | 0.362493 | 0.353950 |
| 10       | 1.5   | First-order         |  |          |          |          |          |          |
| 9.6      | 2     | (1-parameter)       |  | 0.137390 | ---      | 10       | 2.155937 | 1.742451 |
| 8.7      | 2.5   | (2-parameter)       |  | 0.179518 | ---      | 13.00213 | 0.874966 | 1.846968 |
| 8.4      | 3     | Monod Kinetics      |  |          |          |          |          |          |
| 7.4      | 4     | (2-parameter)       |  | 0.447680 | -2.89764 | 10       | 0.482488 | ERR      |
| 6.7      | 5     | (3-parameter)       |  | 0.603190 | -2.28648 | 10.5733  | 0.266507 | ERR      |
| 4.9      | 6     |                     |  |          |          |          |          |          |
| 4.4      | 7     |                     |  |          |          |          |          |          |
| 2.4      | 8     |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |

E-71

\* simultaneous biodegradation with data sets #5A & #5C extracted from Table 7.



Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Naik Thesis (data set #5C) \*;

Substrate : 2,6-dichlorophenol  
Culture : phenol-acclimated sludge  
Condition : 25C & neutral pH

Num.pts.= 18

| Raw Data |       | Summary of results: |  |          |          |          |                   |
|----------|-------|---------------------|--|----------|----------|----------|-------------------|
| S(ppm)   | t(hr) | Kinetic Model       |  | k        | K        | So       | avg dt^2 avg dS^2 |
| 8.5      | 0     | Zero-order          |  |          |          |          |                   |
| 9.3      | 0.5   | (1-parameter)       |  | 0.280787 | ---      | 8.5      | 158.4362 12.49136 |
| 8.7      | 1     | (2-parameter)       |  | 0.317283 | ---      | 11.64680 | 60.92803 6.133543 |
| 9.6      | 1.5   | First-order         |  |          |          |          |                   |
| 9.5      | 2     | (1-parameter)       |  | 0.054667 | ---      | 8.5      | 145.4104 12.37436 |
| 9.3      | 2.5   | (2-parameter)       |  | 0.069822 | ---      | 16.08517 | 65.62941 19.19439 |
| 9.4      | 3     | Monod Kinetics      |  |          |          |          |                   |
| 9.2      | 4     | (2-parameter)       |  | -0.20104 | -8.24788 | 8.5      | 139.1981 18.58435 |
| 9.2      | 5     | (3-parameter)       |  | 0.177265 | -2.14568 | 10.9194  | 59.73697 3.790883 |
| 9.5      | 6     |                     |  |          |          |          |                   |
| 9.2      | 7     |                     |  |          |          |          |                   |
| 9        | 8     |                     |  |          |          |          |                   |
| 9.3      | 20    |                     |  |          |          |          |                   |
| 9.3      | 23    |                     |  |          |          |          |                   |
| 9.4      | 24    |                     |  |          |          |          |                   |
| 6.1      | 26    |                     |  |          |          |          |                   |
| 3.2      | 28    |                     |  |          |          |          |                   |
| 1.5      | 29    |                     |  |          |          |          |                   |
| NA       | NA    |                     |  |          |          |          |                   |
| NA       | NA    |                     |  |          |          |          |                   |
| NA       | NA    |                     |  |          |          |          |                   |
| NA       | NA    |                     |  |          |          |          |                   |
| NA       | NA    |                     |  |          |          |          |                   |
| NA       | NA    |                     |  |          |          |          |                   |
| NA       | NA    |                     |  |          |          |          |                   |

\* simultaneous biodegradation with data sets #5A & #5B extracted from Table 7.

.....

Substrate : phenol  
Culture : phenol-acclimated sludge  
Condition : 25C & neutral pH

Num.pts.= 5

[illegible]

\* simultaneous biodegradation with data sets #6B &6C extracted from Table 8.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Naik Thesis (data set #6B)\*;

Substrate : nitrobenzene  
Culture : phenol-acclimated sludge  
Condition : 25C & neutral pH

Num.pts.= 12

| Raw Data |       | Summary of results: |          |          |          |                     |                     |
|----------|-------|---------------------|----------|----------|----------|---------------------|---------------------|
| S(ppm)   | t(hr) | Kinetic Model       | k        | K        | So       | avg dt <sup>2</sup> | avg dS <sup>2</sup> |
| 10.5     | 0     | Zero-order          |          |          |          |                     |                     |
| 10.1     | 0.5   | (1-parameter)       | 0.940005 | ---      | 10.5     | 0.455324            | 0.402329            |
| 9.9      | 1     | (2-parameter)       | 1.083978 | ---      | 11.32509 | 0.180669            | 0.212288            |
| 10       | 1.5   | First-order         |          |          |          |                     |                     |
| 9.6      | 2     | (1-parameter)       | 0.157258 | ---      | 10.5     | 1.807303            | 1.849040            |
| 8.9      | 2.5   | (2-parameter)       | 0.201894 | ---      | 13.82401 | 0.729827            | 2.051302            |
| 8.6      | 3     | Monod Kinetics      |          |          |          |                     |                     |
| 7.4      | 4     | (2-parameter)       | 0.569914 | -2.49438 | 10.5     | 0.196828            | ERR                 |
| 6.3      | 5     | (3-parameter)       | 0.709233 | -1.98875 | 10.9524  | 0.102240            | ERR                 |
| 4.9      | 6     |                     |          |          |          |                     |                     |
| 3.7      | 7     |                     |          |          |          |                     |                     |
| 2.1      | 8     |                     |          |          |          |                     |                     |
| NA       | NA    |                     |          |          |          |                     |                     |
| NA       | NA    |                     |          |          |          |                     |                     |
| NA       | NA    |                     |          |          |          |                     |                     |
| NA       | NA    |                     |          |          |          |                     |                     |
| NA       | NA    |                     |          |          |          |                     |                     |
| NA       | NA    |                     |          |          |          |                     |                     |
| NA       | NA    |                     |          |          |          |                     |                     |
| NA       | NA    |                     |          |          |          |                     |                     |
| NA       | NA    |                     |          |          |          |                     |                     |
| NA       | NA    |                     |          |          |          |                     |                     |
| NA       | NA    |                     |          |          |          |                     |                     |
| NA       | NA    |                     |          |          |          |                     |                     |
| NA       | NA    |                     |          |          |          |                     |                     |
| NA       | NA    |                     |          |          |          |                     |                     |
| NA       | NA    |                     |          |          |          |                     |                     |

E-74

\* simultaneous biodegradation with data sets #6A & #6C extracted from Table 8.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Naik Thesis (data set #6C)\*;

Substrate : 2,6-dichlorophenol  
Culture : phenol-acclimated sludge  
Condition : 25C & neutral pH

Num.pts.= 18

| Raw Data |       | Summary of results: |  |          |          |          |          |          |
|----------|-------|---------------------|--|----------|----------|----------|----------|----------|
| S(ppm)   | t(hr) | Kinetic Model       |  | k        | K        | So       | avg dt^2 | avg dS^2 |
| 8.7      | 0     | Zero-order          |  |          |          |          |          |          |
| 8.8      | 0.5   | (1-parameter)       |  | 0.200631 | ---      | 8.7      | 87.26253 | 3.512567 |
| 8.7      | 1     | (2-parameter)       |  | 0.269520 | ---      | 10.51909 | 50.59374 | 3.675206 |
| 8.6      | 1.5   | First-order         |  |          |          |          |          |          |
| 8.7      | 2     | (1-parameter)       |  | 0.045895 | ---      | 8.7      | 104.1847 | 6.187599 |
| 8.6      | 2.5   | (2-parameter)       |  | 0.063021 | ---      | 13.86741 | 58.25049 | 11.29282 |
| 8.7      | 3     | Monod Kinetics      |  |          |          |          |          |          |
| 8.6      | 4     | (2-parameter)       |  | 0.047528 | -3.59601 | 8.7      | 62.65973 | 2.255615 |
| 8.6      | 5     | (3-parameter)       |  | 0.067093 | -3.46826 | 9.3069   | 40.24882 | 2.058307 |
| 8.6      | 6     |                     |  |          |          |          |          |          |
| 8.5      | 7     |                     |  |          |          |          |          |          |
| 8.2      | 8     |                     |  |          |          |          |          |          |
| 8.2      | 20    |                     |  |          |          |          |          |          |
| 8.4      | 23    |                     |  |          |          |          |          |          |
| 8.3      | 24    |                     |  |          |          |          |          |          |
| 5.7      | 26    |                     |  |          |          |          |          |          |
| 2.4      | 28    |                     |  |          |          |          |          |          |
| 1.7      | 29    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |

E-75

\* simultaneous biodegradation with data sets #6A & #6B extracted from Table 8.

---

Substrate : 2-chlorophenol  
Culture : unacclimated sludge  
Condition : 27C & neutral pH

Condition : 27C & neutral pH

E-76

\* simultaneous biodegradation with data sets #7B & #7C extracted from Table 9.

---

Substrate : nitrobenzene  
Culture : unacclimated sludge  
Condition : 27C & neutral pH

Num.pts.= 7

[illegible]

E-77

\* simultaneous biodegradation with data sets #7A & #7C extracted from Table 9.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Naik Thesis (data set #7C)\*;

Substrate : 2,6-dichlorophenol  
Culture : unacclimated sludge  
Condition : 27C & neutral pH

Num.pts.= 19

| Raw Data |       | Summary of results: |  |          |          |          |          |          |
|----------|-------|---------------------|--|----------|----------|----------|----------|----------|
| S(ppm)   | t(hr) | Kinetic Model       |  | k        | K        | So       | avg dt^2 | avg dS^2 |
| 8.3      | 0     | Zero-order          |  |          |          |          |          |          |
| 8.3      | 1     | (1-parameter)       |  | 0.074892 | ---      | 8.3      | 1204.173 | 6.754137 |
| 8.1      | 2     | (2-parameter)       |  | 0.116455 | ---      | 11.39479 | 591.9280 | 8.027660 |
| 7.9      | 3     | First-order         |  |          |          |          |          |          |
| 8.3      | 4     | (1-parameter)       |  | 0.020285 | ---      | 8.3      | 1315.907 | 12.20369 |
| 8.2      | 5     | (2-parameter)       |  | 0.031891 | ---      | 20.09035 | 630.4904 | 49.68160 |
| 8.1      | 6     | Monod Kinetics      |  |          |          |          |          |          |
| 8.4      | 7     | (2-parameter)       |  | 0.032742 | -2.30610 | 8.3      | 1148.872 | 3.368582 |
| 8.1      | 22    | (3-parameter)       |  | 0.056433 | -2.08646 | 10.194   | 577.0148 | 3.942102 |
| 8.3      | 27    |                     |  |          |          |          |          |          |
| 8.6      | 33    |                     |  |          |          |          |          |          |
| 8.7      | 44    |                     |  |          |          |          |          |          |
| 8.5      | 49    |                     |  |          |          |          |          |          |
| 8.4      | 57    |                     |  |          |          |          |          |          |
| 8.4      | 68    |                     |  |          |          |          |          |          |
| 7.8      | 70    |                     |  |          |          |          |          |          |
| 6.6      | 73    |                     |  |          |          |          |          |          |
| 3.5      | 76    |                     |  |          |          |          |          |          |
| 1.1      | 79    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |

\* simultaneous biodegradation with data sets #7A & #7B extracted from Table 9.

---

Substrate : 2-chlorophenol  
Culture : unacclimated sludge  
Condition : 27C & neutral pH

Condition : 27C & neutral pH

E-79

\* simultaneous biodegradation with data sets #8B & #8C extracted from Table 10.



---

Substrate : nitrobenzene  
Culture : unacclimated sludge  
Condition : 27C & neutral pH

Num.pts.= 8

[illegible]

\* simultaneous biodegradation with data sets #8A & #8C extracted from Table 10.

# Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Naik Thesis (data set #8C)\*;

Substrate : 2,6-dichlorophenol  
Culture : unacclimated sludge  
Condition : 27C & neutral pH

Num.pts.= 15

| Raw Data |       | Summary of results: |          |          |          |          |          |
|----------|-------|---------------------|----------|----------|----------|----------|----------|
| S(ppm)   | t(hr) | Kinetic Model       | k        | K        | So       | avg dt^2 | avg dS^2 |
| 8.3      | 0     | Zero-order          |          |          |          |          |          |
| 7.7      | 1     | (1-parameter)       | 0.163623 | ---      | 8.3      | 70.20185 | 1.879479 |
| 8.1      | 2     | (2-parameter)       | 0.220579 | ---      | 9.752036 | 43.55886 | 2.119371 |
| 7.9      | 3     | First-order         |          |          |          |          |          |
| 8.4      | 4     | (1-parameter)       | 0.034780 | ---      | 8.3      | 103.8449 | 3.226772 |
| 8.2      | 5     | (2-parameter)       | 0.050517 | ---      | 12.55779 | 57.68581 | 6.659998 |
| 8.1      | 6     | Monod Kinetics      |          |          |          |          |          |
| 8        | 7     | (2-parameter)       | 0.054939 | -3.40626 | 8.3      | 42.25134 | 1.404490 |
| 7.9      | 22    | (3-parameter)       | 0.072646 | -3.26381 | 8.842    | 31.25375 | 1.277718 |
| 7.1      | 23    |                     |          |          |          |          |          |
| 6.2      | 25    |                     |          |          |          |          |          |
| 5.3      | 26    |                     |          |          |          |          |          |
| 4.2      | 27    |                     |          |          |          |          |          |
| 3.1      | 28    |                     |          |          |          |          |          |
| 1.9      | 29    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |          |

E-01

\* simultaneous biodegradation with data sets #8A & #8B extracted from Table 10.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Naik Thesis (data set #9A)\*;

Substrate : 2-chlorophenol  
Culture : unacclimated sludge  
Condition : 27C & neutral pH

Num.pts.= 11

| Raw Data |       | Summary of results: |  |          |          |          |                     |                     |
|----------|-------|---------------------|--|----------|----------|----------|---------------------|---------------------|
| S(ppm)   | t(hr) | Kinetic Model       |  | k        | K        | So       | avg dt <sup>2</sup> | avg dS <sup>2</sup> |
| 19.6     | 0     | Zero-order          |  |          |          |          |                     |                     |
| 18.3     | 1     | (1-parameter)       |  | 0.671561 | ---      | 19.6     | 34.87854            | 15.73006            |
| 15.7     | 2     | (2-parameter)       |  | 0.494106 | ---      | 16.74106 | 25.53568            | 6.234312            |
| 14.8     | 3     | First-order         |  |          |          |          |                     |                     |
| 13.5     | 4     | (1-parameter)       |  | 0.053720 | ---      | 19.6     | 14.49138            | 5.359554            |
| 11.5     | 5     | (2-parameter)       |  | 0.045026 | ---      | 16.71778 | 9.749246            | 2.958827            |
| 10.3     | 6     | Monod Kinetics      |  |          |          |          |                     |                     |
| 9.4      | 7     | (2-parameter)       |  | -0.46727 | -20.4081 | 19.6     | 4.065799            | 1.045544            |
| 7        | 22    | (3-parameter)       |  | -0.44116 | -19.7274 | ERR      | 4.030865            | ERR                 |
| 5.6      | 27    |                     |  |          |          |          |                     |                     |
| 4.1      | 33    |                     |  |          |          |          |                     |                     |
| NA       | NA    |                     |  |          |          |          |                     |                     |
| NA       | NA    |                     |  |          |          |          |                     |                     |
| NA       | NA    |                     |  |          |          |          |                     |                     |
| NA       | NA    |                     |  |          |          |          |                     |                     |
| NA       | NA    |                     |  |          |          |          |                     |                     |
| NA       | NA    |                     |  |          |          |          |                     |                     |
| NA       | NA    |                     |  |          |          |          |                     |                     |
| NA       | NA    |                     |  |          |          |          |                     |                     |
| NA       | NA    |                     |  |          |          |          |                     |                     |
| NA       | NA    |                     |  |          |          |          |                     |                     |
| NA       | NA    |                     |  |          |          |          |                     |                     |
| NA       | NA    |                     |  |          |          |          |                     |                     |
| NA       | NA    |                     |  |          |          |          |                     |                     |
| NA       | NA    |                     |  |          |          |          |                     |                     |
| NA       | NA    |                     |  |          |          |          |                     |                     |
| NA       | NA    |                     |  |          |          |          |                     |                     |

E-82

\* simultaneous biodegradation with data sets #9B & #9C extracted from Table 11.

[illegible]

Substrate : nitrobenzene  
Culture : unacclimated sludge  
Condition : 27C & neutral pH

Num.pts.= 7

[illegible]

7-8 (3)

\* simultaneous biodegradation with data sets #9A & #9C extracted from Table 11.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Naik Thesis (data set #9C)\*;

Substrate : 2,6-dichlorophenol  
Culture : unacclimated sludge  
Condition : 27C & neutral pH

Num.pts.= 19

| Raw Data |       | Summary of results: |          |          |          |                     |                     |
|----------|-------|---------------------|----------|----------|----------|---------------------|---------------------|
| S(ppm)   | t(hr) | Kinetic Model       | k        | K        | So       | avg dt <sup>2</sup> | avg dS <sup>2</sup> |
| 8.6      | 0     | Zero-order          |          |          |          |                     |                     |
| 8.5      | 1     | (1-parameter)       | 0.068792 | ---      | 8.6      | 1056.731            | 5.000908            |
| 8.4      | 2     | (2-parameter)       | 0.106109 | ---      | 11.23285 | 550.5479            | 6.198702            |
| 8.5      | 3     | First-order         |          |          |          |                     |                     |
| 8.3      | 4     | (1-parameter)       | 0.017272 | ---      | 8.6      | 1229.167            | 9.832323            |
| 8.6      | 5     | (2-parameter)       | 0.027164 | ---      | 17.80298 | 606.2212            | 32.67928            |
| 8.2      | 6     | Monod Kinetics      |          |          |          |                     |                     |
| 8.4      | 7     | (2-parameter)       | 0.021373 | -3.11778 | 8.6      | 888.7513            | 2.240918            |
| 8.7      | 22    | (3-parameter)       | 0.036604 | -2.88605 | 9.8041   | 505.6305            | 2.454720            |
| 8.4      | 27    |                     |          |          |          |                     |                     |
| 8.6      | 33    |                     |          |          |          |                     |                     |
| 8.7      | 44    |                     |          |          |          |                     |                     |
| 8.5      | 49    |                     |          |          |          |                     |                     |
| 8.5      | 57    |                     |          |          |          |                     |                     |
| 8.4      | 68    |                     |          |          |          |                     |                     |
| 7.8      | 70    |                     |          |          |          |                     |                     |
| 6.7      | 73    |                     |          |          |          |                     |                     |
| 3.8      | 76    |                     |          |          |          |                     |                     |
| 1.4      | 79    |                     |          |          |          |                     |                     |
| NA       | NA    |                     |          |          |          |                     |                     |
| NA       | NA    |                     |          |          |          |                     |                     |
| NA       | NA    |                     |          |          |          |                     |                     |
| NA       | NA    |                     |          |          |          |                     |                     |
| NA       | NA    |                     |          |          |          |                     |                     |
| NA       | NA    |                     |          |          |          |                     |                     |

E-84

\* simultaneous biodegradation with data sets #9A & #9B extracted from Table 11.

.....

Substrate : 2-chlorophenol  
Culture : unacclimated sludge  
Condition : 27C & neutral pH

Summary of results:

E-85

\* simultaneous biodegradation with data sets #10B & #10C extracted from Table 12.

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98-7

\* simultaneous biodegradation with data sets #10A & #10C extracted from Table 12.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Naik Thesis (data set #10C)\*;

Substrate : 2,6-dichlorophenol  
Culture : unacclimated sludge  
Condition : 27C & neutral pH

Num.pts.= 15

| Raw Data |       | Summary of results: |          |          |          |          |          |  |
|----------|-------|---------------------|----------|----------|----------|----------|----------|--|
| S(ppm)   | t(hr) | Kinetic Model       | k        | K        | So       | avg dt^2 | avg dS^2 |  |
| 9.3      | 0     | Zero-order          |          |          |          |          |          |  |
| 8.7      | 1     | (1-parameter)       | 0.192392 | ---      | 9.3      | 71.84016 | 2.659150 |  |
| 8.9      | 2     | (2-parameter)       | 0.259892 | ---      | 10.97050 | 47.30081 | 3.194885 |  |
| 8.9      | 3     | First-order         |          |          |          |          |          |  |
| 9        | 4     | (1-parameter)       | 0.039339 | ---      | 9.3      | 111.7327 | 4.892775 |  |
| 8.8      | 5     | (2-parameter)       | 0.058323 | ---      | 15.20294 | 62.84236 | 12.23303 |  |
| 8.9      | 6     | Monod Kinetics      |          |          |          |          |          |  |
| 8.8      | 7     | (2-parameter)       | 0.072315 | -3.39644 | 9.3      | 44.69114 | 1.958201 |  |
| 8.9      | 22    | (3-parameter)       | 0.095123 | -3.21504 | 9.91     | 36.01829 | 1.854714 |  |
| 8.1      | 23    |                     |          |          |          |          |          |  |
| 7        | 25    |                     |          |          |          |          |          |  |
| 5.7      | 26    |                     |          |          |          |          |          |  |
| 4.5      | 27    |                     |          |          |          |          |          |  |
| 3.3      | 28    |                     |          |          |          |          |          |  |
| 1.7      | 29    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |

E-87

\* simultaneous biodegradation with data sets #10A & #10B extracted from Table 12.



.....

Substrate : nitrobenzene  
Culture : phenol-acclimated sludge  
Condition : 27C & neutral pH

Num.pts.= 6

[illegible]

\* simultaneous biodegradation with data sets #11A & #11C extracted from Table 13.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Naik Thesis (data set #11C)\*;

Substrate : 2,6-dichlorophenol  
Culture : phenol-acclimated sludge  
Condition : 27C & neutral pH

Num.pts.= 16

| Raw Data |       | Summary of results: |  |          |          |          |          |          |
|----------|-------|---------------------|--|----------|----------|----------|----------|----------|
| S(ppm)   | t(hr) | Kinetic Model       |  | k        | K        | So       | avg dt^2 | avg dS^2 |
| 8.9      | 0     | Zero-order          |  |          |          |          |          |          |
| 8.8      | 0.25  | (1-parameter)       |  | 0.162976 | ---      | 8.9      | 155.1395 | 4.120722 |
| 8.5      | 0.5   | (2-parameter)       |  | 0.227158 | ---      | 10.89109 | 98.15956 | 5.065136 |
| 8.6      | 1     | First-order         |  |          |          |          |          |          |
| 8.8      | 1.5   | (1-parameter)       |  | 0.039936 | ---      | 8.9      | 201.2577 | 8.173038 |
| 8.8      | 2     | (2-parameter)       |  | 0.058221 | ---      | 16.17914 | 115.8518 | 24.99725 |
| 8.4      | 4     | Monod Kinetics      |  |          |          |          |          |          |
| 8.8      | 6     | (2-parameter)       |  | 0.053264 | -3.10254 | 8.9      | 114.1121 | 2.424689 |
| 8.6      | 9     | (3-parameter)       |  | 0.077399 | -2.90979 | 9.6825   | 83.53555 | 2.390878 |
| 8.8      | 22    |                     |  |          |          |          |          |          |
| 8.6      | 26    |                     |  |          |          |          |          |          |
| 8.2      | 28    |                     |  |          |          |          |          |          |
| 7.6      | 30    |                     |  |          |          |          |          |          |
| 5.9      | 32    |                     |  |          |          |          |          |          |
| 2.9      | 34    |                     |  |          |          |          |          |          |
| 1.3      | 36    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |
| NA       | NA    |                     |  |          |          |          |          |          |

\* simultaneous biodegradation with data sets #11A & #11B extracted from Table 13.

---

Substrate : nitrobenzene  
Culture : phenol-acclimated sludge  
Condition : 27C & neutral pH

Substrate : nitrobenzene  
Culture : phenol-acclimated sludge  
Condition : 27C & neutral pH

E-90

\* simultaneous biodegradation with data sets #12A & #12C extracted from Table 14.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Naik Thesis (data set #12C)\*;

Substrate : 2,6-dichlorophenol  
Culture : phenol-acclimated sludge  
Condition : 27C & neutral pH

Num.pts.= 16

| Raw Data |       | Summary of results: |  |          |          |          |                     |                     |
|----------|-------|---------------------|--|----------|----------|----------|---------------------|---------------------|
| S(ppm)   | t(hr) | Kinetic Model       |  | k        | K        | So       | avg dt <sup>2</sup> | avg dS <sup>2</sup> |
| 7.9      | 0     | Zero-order          |  |          |          |          |                     |                     |
| 7.9      | 0.25  | (1-parameter)       |  | 0.142676 | ---      | 7.9      | 140.2959            | 2.855952            |
| 8        | 0.5   | (2-parameter)       |  | 0.191370 | ---      | 9.602857 | 78.17644            | 2.863019            |
| 8.1      | 1     | First-order         |  |          |          |          |                     |                     |
| 7.8      | 1.5   | (1-parameter)       |  | 0.040931 | ---      | 7.9      | 196.8793            | 6.303868            |
| 8.2      | 2     | (2-parameter)       |  | 0.058100 | ---      | 14.41952 | 107.6878            | 18.00496            |
| 8.1      | 4     | Monod Kinetics      |  |          |          |          |                     |                     |
| 8        | 6     | (2-parameter)       |  | 0.058009 | -2.40330 | 7.9      | 106.5933            | 1.727494            |
| 7.9      | 9     | (3-parameter)       |  | 0.075330 | -2.39674 | 8.7398   | 59.02954            | 1.602217            |
| 7.8      | 22    |                     |  |          |          |          |                     |                     |
| 7.6      | 26    |                     |  |          |          |          |                     |                     |
| 7.2      | 28    |                     |  |          |          |          |                     |                     |
| 5.8      | 30    |                     |  |          |          |          |                     |                     |
| 4.9      | 32    |                     |  |          |          |          |                     |                     |
| 3        | 34    |                     |  |          |          |          |                     |                     |
| 1        | 36    |                     |  |          |          |          |                     |                     |
| NA       | NA    |                     |  |          |          |          |                     |                     |
| NA       | NA    |                     |  |          |          |          |                     |                     |
| NA       | NA    |                     |  |          |          |          |                     |                     |
| NA       | NA    |                     |  |          |          |          |                     |                     |
| NA       | NA    |                     |  |          |          |          |                     |                     |
| NA       | NA    |                     |  |          |          |          |                     |                     |
| NA       | NA    |                     |  |          |          |          |                     |                     |
| NA       | NA    |                     |  |          |          |          |                     |                     |
| NA       | NA    |                     |  |          |          |          |                     |                     |

\* simultaneous biodegradation with data sets #12A & #12B extracted from Table 14.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Pak Thesis (data set #1)\* ;

Substrate : 2,6-dichlorophenol  
Culture : mlsa (acclimated sludge)  
Condition : 23C & pH 7.5-7.6

Num.pts.= 11

| Raw Data |       | Summary of results: |          |          |          |          |          |  |
|----------|-------|---------------------|----------|----------|----------|----------|----------|--|
| S(ppm)   | t(hr) | Kinetic Model       | k        | K        | So       | avg dt^2 | avg dS^2 |  |
| 9.59     | 0     | Zero-order          |          |          |          |          |          |  |
| 8.99     | 2     | (1-parameter)       | 0.159131 | ---      | 9.59     | 48.44946 | 1.226881 |  |
| 8.76     | 4     | (2-parameter)       | 0.188185 | ---      | 10.49213 | 37.34534 | 1.322538 |  |
| 8.44     | 6     | First-order         |          |          |          |          |          |  |
| 8.37     | 8     | (1-parameter)       | 0.085090 | ---      | 9.59     | 249.6165 | 16.68944 |  |
| 6.96     | 23    | (2-parameter)       | 0.128862 | ---      | 53.81297 | 104.7477 | 369.9849 |  |
| 6.9      | 25    | Monod Kinetics      |          |          |          |          |          |  |
| 6.87     | 27    | (2-parameter)       | 0.099495 | -1.00907 | 9.59     | 6.191295 | 1.507085 |  |
| 6.56     | 29    | (3-parameter)       | 0.086566 | -1.08023 | 9.2841   | 3.703227 | 1.743724 |  |
| 5.88     | 31    |                     |          |          |          |          |          |  |
| 0.08     | 47    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |

\* corresponds to data extracted from Table 16 on page 39.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Variable Biomass

Data source -- Pak Thesis (data set #1) \*;

Substrate : 2,6-dichlorophenol  
Culture : mlsa (acclimated sludge)  
Condition : 23C & pH 7.5-7.6

Num.pts.= 11

| Raw Data |       | Summary of results: |          |          |          |          |
|----------|-------|---------------------|----------|----------|----------|----------|
| S(ppm)   | t(hr) | Kinetic Model       | ko       | K        | avg dt^2 | avg dS^2 |
| 9.59     | 0     | Zero-order          |          |          |          |          |
| 8.99     | 2     | (1-parameter)       | 0.000039 | ---      | 53.12666 | 1.320622 |
| 8.76     | 4     | First-order         |          |          |          |          |
| 8.44     | 6     | (1-parameter)       | 0.000021 | ---      | 255.2972 | 17.28635 |
| 8.37     | 8     | Monod Kinetics      |          |          |          |          |
| 6.96     | 23    | (2-parameter)       | 0.000023 | -1.01247 | 6.038392 | 1.561244 |
| 6.9      | 25    |                     |          |          |          |          |
| 6.87     | 27    |                     |          |          |          |          |
| 6.56     | 29    |                     |          |          |          |          |
| 5.88     | 31    |                     |          |          |          |          |
| 0.08     | 47    |                     |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |

Bo = 4250 ppm \*\*

Yc = -41.3 \*\*

\* corresponds to data extracted from Table 16 on page 39.

\*\*estimated from available MLSS measurements.

.....

Substrate : 2,6-dichlorophenol  
Culture : mlss (acclimated sludge)  
Condition : 24C & pH 7.3-7.4

Num.pts.= 6

[illegible]

E-94

\* corresponds to data extracted from Table 17 on page 39.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Pak Thesis (data set #3)\*;

Substrate : 2,6-dichlorophenol  
Culture : m1ss (unacclimated sludge)  
Condition : 25C & pH 7.9-8.1

Num.pts.= 20

| Raw Data |       | Summary of results: |          |          |          |                     |                     |
|----------|-------|---------------------|----------|----------|----------|---------------------|---------------------|
| S(ppm)-  | t(hr) | Kinetic Model       | k        | K        | So       | avg dt <sup>2</sup> | avg dS <sup>2</sup> |
| 10.83    | 0     | Zero-order          |          |          |          |                     |                     |
| 10.59    | 2     | (1-parameter)       | 0.103428 | ---      | 10.83    | 22.94821            | 0.245485            |
| 10.13    | 4     | (2-parameter)       | 0.095454 | ---      | 10.38416 | 17.21855            | 0.156885            |
| 9.66     | 6     | First-order         |          |          |          |                     |                     |
| 9.04     | 8     | (1-parameter)       | 0.014974 | ---      | 10.83    | 32.44005            | 0.156949            |
| 8.22     | 24    | (2-parameter)       | 0.015821 | ---      | 11.38486 | 29.05011            | 0.209786            |
| 8.11     | 26    | Monod Kinetics      |          |          |          |                     |                     |
| 7.58     | 28    | (2-parameter)       | 0.167916 | 4.354853 | 10.83    | 16.72815            | 0.131351            |
| 7.46     | 30    | (3-parameter)       | 0.130604 | 2.282173 | 10.5251  | 15.28118            | 0.118479            |
| 6.73     | 32    |                     |          |          |          |                     |                     |
| 5.24     | 48    |                     |          |          |          |                     |                     |
| 5.27     | 50    |                     |          |          |          |                     |                     |
| 5.25     | 52    |                     |          |          |          |                     |                     |
| 4.91     | 54    |                     |          |          |          |                     |                     |
| 4.77     | 56    |                     |          |          |          |                     |                     |
| 4.2      | 72    |                     |          |          |          |                     |                     |
| 3.98     | 74    |                     |          |          |          |                     |                     |
| 3.54     | 76    |                     |          |          |          |                     |                     |
| 3.35     | 78    |                     |          |          |          |                     |                     |
| 2.46     | 80    |                     |          |          |          |                     |                     |
| NA       | NA    |                     |          |          |          |                     |                     |
| NA       | NA    |                     |          |          |          |                     |                     |
| NA       | NA    |                     |          |          |          |                     |                     |
| NA       | NA    |                     |          |          |          |                     |                     |
| NA       | NA    |                     |          |          |          |                     |                     |

E-95

\* corresponds to data extracted from Table 12 on page 37.



Regression of Batch-Reactor Biodegradation Data (with respect to time) : Variable Biomass

Data source -- Pak Thesis (data set #3)\*;

Substrate : 2,6-dichlorophenol  
Culture : m1ss (unacclimated sludge)  
Condition : 25C & pH 7.9-8.1

Num.pts.= 20

| Raw Data |       | Summary of results: |          |          |          |          |
|----------|-------|---------------------|----------|----------|----------|----------|
| S(ppm)   | t(hr) | Kinetic Model       | ko       | K        | avg dt^2 | avg dS^2 |
| 10.83    | 0     | Zero-order          |          |          |          |          |
| 10.59    | 2     | (1-parameter)       | 0.000027 | ---      | 20.96710 | 0.217376 |
| 10.13    | 4     | First-order         |          |          |          |          |
| 9.66     | 6     | (1-parameter)       | 0.000004 | ---      | 36.18287 | 0.172644 |
| 9.04     | 8     | Monod Kinetics      |          |          |          |          |
| 8.22     | 24    | (2-parameter)       | 0.000041 | 3.278566 | 16.47538 | 0.130955 |
| 8.11     | 26    |                     |          |          |          |          |
| 7.58     | 28    |                     |          |          |          |          |
| 7.46     | 30    |                     |          |          |          |          |
| 6.73     | 32    |                     |          |          |          |          |
| 5.24     | 48    |                     |          |          |          |          |
| 5.27     | 50    |                     |          |          |          |          |
| 5.25     | 52    |                     |          |          |          |          |
| 4.91     | 54    |                     |          |          |          |          |
| 4.77     | 56    |                     |          |          |          |          |
| 4.2      | 72    |                     |          |          |          |          |
| 3.98     | 74    |                     |          |          |          |          |
| 3.54     | 76    |                     |          |          |          |          |
| 3.35     | 78    |                     |          |          |          |          |
| 2.46     | 80    |                     |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |
| NA       | NA    |                     |          |          |          |          |

Bo = 3830 ppm \*\*

Yc = -36.5 \*\*

\* corresponds to data extracted from Table 12 on page 37.

\*\*estimated from available MLSS measurements.

-----

Substrate : 2,6-dichlorophenol  
Culture : mlss (unacclimated sludge)  
Condition : 23C & pH 6.7-6.9

Num.pts.= 5

[illegible]

\* corresponds to data extracted from Table 13 on page 37.

---

Substrate : 2-chlorophenol  
Culture : mss (acclimated sludge)  
Condition : 25C & pH 7.8-8.0

Num.pts.= 5

[illegible]

E-98

\* corresponds to data extracted from Table 9 on page 35.

.....

Substrate : 2-chlorophenol  
Culture : mss (acclimated sludge)  
Condition : 25C & pH 7.8-8.0

Num.pts.= 5

[illegible]

Bo = 3920 ppm \*\* \* corresponds to data extracted from Table 9 on page 35.  
Yc = -9.6 \*\* \*\*estimated from available MLSS measurements.

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 92 93 94 95 96 97 98 99 100 101 102 103 104 105 106 107 108 109 110 111 112 113 114 115 116 117 118 119 120 121 122 123 124 125 126 127 128 129 130 131 132 133 134 135 136 137 138 139 140 141 142 143 144 145 146 147 148 149 150 151 152 153 154 155 156 157 158 159 160 161 162 163 164 165 166 167 168 169 170 171 172 173 174 175 176 177 178 179 180 181 182 183 184 185 186 187 188 189 190 191 192 193 194 195 196 197 198 199 200 201 202 203 204 205 206 207 208 209 210 211 212 213 214 215 216 217 218 219 220 221 222 223 224 225 226 227 228 229 230 231 232 233 234 235 236 237 238 239 240 241 242 243 244 245 246 247 248 249 250 251 252 253 254 255 256 257 258 259 260 261 262 263 264 265 266 267 268 269 270 271 272 273 274 275 276 277 278 279 280 281 282 283 284 285 286 287 288 289 290 291 292 293 294 295 296 297 298 299 300 301 302 303 304 305 306 307 308 309 310 311 312 313 314 315 316 317 318 319 320 321 322 323 324 325 326 327 328 329 330 331 332 333 334 335 336 337 338 339 340 341 342 343 344 345 346 347 348 349 350 351 352 353 354 355 356 357 358 359 360 361 362 363 364 365 366 367 368 369 370 371 372 373 374 375 376 377 378 379 380 381 382 383 384 385 386 387 388 389 390 391 392 393 394 395 396 397 398 399 400 401 402 403 404 405 406 407 408 409 410 411 412 413 414 415 416 417 418 419 420 421 422 423 424 425 426 427 428 429 430 431 432 433 434 435 436 437 438 439 440 441 442 443 444 445 446 447 448 449 450 451 452 453 454 455 456 457 458 459 460 461 462 463 464 465 466 467 468 469 470 471 472 473 474 475 476 477 478 479 480 481 482 483 484 485 486 487 488 489 490 491 492 493 494 495 496 497 498 499 500 501 502 503 504 505 506 507 508 509 510 511 512 513 514 515 516 517 518 519 520 521 522 523 524 525 526 527 528 529 530 531 532 533 534 535 536 537 538 539 540 541 542 543 544 545 546 547 548 549 550 551 552 553 554 555 556 557 558 559 560 561 562 563 564 565 566 567 568 569 570 571 572 573 574 575 576 577 578 579 580 581 582 583 584 585 586 587 588 589 590 591 592 593 594 595 596 597 598 599 600 601 602 603 604 605 606 607 608 609 610 611 612 613 614 615 616 617 618 619 620 621 622 623 624 625 626 627 628 629 630 631 632 633 634 635 636 637 638 639 640 641 642 643 644 645 646 647 648 649 650 651 652 653 654 655 656 657 658 659 660 661 662 663 664 665 666 667 668 669 670 671 672 673 674 675 676 677 678 679 680 681 682 683 684 685 686 687 688 689 690 691 692 693 694 695 696 697 698 699 700 701 702 703 704 705 706 707 708 709 710 711 712 713 714 715 716 717 718 719 720 721 722 723 724 725 726 727 728 729 730 731 732 733 734 735 736 737 738 739 740 741 742 743 744 745 746 747 748 749 750 751 752 753 754 755 756 757 758 759 760 761 762 763 764 765 766 767 768 769 770 771 772 773 774 775 776 777 778 779 780 781 782 783 784 785 786 787 788 789 790 791 792 793 794 795 796 797 798 799 800 801 802 803 804 805 806 807 808 809 810 811 812 813 814 815 816 817 818 819 820 821 822 823 824 825 826 827 828 829 830 831 832 833 834 835 836 837 838 839 840 841 842 843 844 845 846 847 848 849 850 851 852 853 854 855 856 857 858 859 860 861 862 863 864 865 866 867 868 869 870 871 872 873 874 875 876 877 878 879 880 881 882 883 884 885 886 887 888 889 890 891 892 893 894 895 896 897 898 899 900 901 902 903 904 905 906 907 908 909 910 911 912 913 914 915 916 917 918 919 920 921 922 923 924 925 926 927 928 929 930 931 932 933 934 935 936 937 938 939 940 941 942 943 944 945 946 947 948 949 950 951 952 953 954 955 956 957 958 959 960 961 962 963 964 965 966 967 968 969 970 971 972 973 974 975 976 977 978 979 980 981 982 983 984 985 986 987 988 989 990 991 992 993 994 995 996 997 998 999 1000 1001 1002 1003 1004 1005 1006 1007 1008 1009 1010 1011 1012 1013 1014 1015 1016 1017 1018 1019 1020 1021 1022 1023 1024 1025 1026 1027 1028 1029 1030 1031 1032 1033 1034 1035 1036 1037 1038 1039 1040 1

Substrate : 2-chlorophenol  
Culture : mls (acclimated sludge)  
Condition : 23C & pH 7.8-8.0

Substrate : 2-chlorophenol  
Culture : mls (acclimated sludge)  
Condition : 23C & pH 7.8-8.0

E-100

\* corresponds to data extracted from Table 10 on page 35.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Pak Thesis (data set #7)\*; Substrate : 2-chlorophenol  
Culture : m1ss (unacclimated sludge)  
Condition : 22C & pH 7.4-8.0

Num.pts.= 15

| Raw Data |       | Summary of results: |          |          |          |          |          |  |
|----------|-------|---------------------|----------|----------|----------|----------|----------|--|
| S(ppm)   | t(hr) | Kinetic Model       | k        | K        | So       | avg dt^2 | avg dS^2 |  |
| 18.49    | 0     | Zero-order          |          |          |          |          |          |  |
| 16.5     | 2     | (1-parameter)       | 0.361778 | ---      | 18.49    | 40.86991 | 5.349212 |  |
| 15.58    | 4     | (2-parameter)       | 0.304166 | ---      | 16.38749 | 30.95141 | 2.863530 |  |
| 14.44    | 6     | First-order         |          |          |          |          |          |  |
| 8.77     | 20    | (1-parameter)       | 0.038452 | ---      | 18.49    | 2.841515 | 0.118965 |  |
| 7.77     | 22    | (2-parameter)       | 0.037704 | ---      | 17.95291 | 2.659731 | 0.094932 |  |
| 6.75     | 24    | Monod Kinetics      |          |          |          |          |          |  |
| 6.41     | 26    | (2-parameter)       | -4.51264 | -126.460 | 18.49    | 2.637250 | 0.081260 |  |
| 5.76     | 28    | (3-parameter)       | -6.76925 | -186.950 | 18.1925  | 2.611376 | 0.076964 |  |
| 5.68     | 30    |                     |          |          |          |          |          |  |
| 3.66     | 46    |                     |          |          |          |          |          |  |
| 3        | 48    |                     |          |          |          |          |          |  |
| 2.93     | 50    |                     |          |          |          |          |          |  |
| 2.6      | 52    |                     |          |          |          |          |          |  |
| 2.08     | 54.25 |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |
| NA       | NA    |                     |          |          |          |          |          |  |

E-101

\* corresponds to data extracted from Table 6 on page 33.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Variable Biomass

Data source -- Pak Thesis (data set #7)\*;

Substrate : 2-chlorophenol  
Culture : mlss (unacclimated sludge)  
Condition : 22C & pH 7.4-8.0

Num.pts.= 15

| Raw Data |       | Summary of results: |          |          |                   |
|----------|-------|---------------------|----------|----------|-------------------|
| S(ppm)   | t(hr) | Kinetic Model       | ko       | K        | avg dt^2 avg dS^2 |
| 18.49    | 0     | Zero-order          |          |          |                   |
| 16.5     | 2     | (1-parameter)       | 0.000085 | ---      | 43.84690 6.170249 |
| 15.58    | 4     | First-order         |          |          |                   |
| 14.44    | 6     | (1-parameter)       | 0.000008 | ---      | 3.259970 0.168895 |
| 8.77     | 20    | Monod Kinetics      |          |          |                   |
| 7.77     | 22    | (2-parameter)       | -0.00059 | -76.0320 | 2.632051 0.080671 |
| 6.75     | 24    |                     |          |          |                   |
| 6.41     | 26    |                     |          |          |                   |
| 5.76     | 28    |                     |          |          |                   |
| 5.68     | 30    |                     |          |          |                   |
| 3.66     | 46    |                     |          |          |                   |
| 3        | 48    |                     |          |          |                   |
| 2.93     | 50    |                     |          |          |                   |
| 2.6      | 52    |                     |          |          |                   |
| 2.08     | 54.25 |                     |          |          |                   |
| NA       | NA    |                     |          |          |                   |
| NA       | NA    |                     |          |          |                   |
| NA       | NA    |                     |          |          |                   |
| NA       | NA    |                     |          |          |                   |
| NA       | NA    |                     |          |          |                   |
| NA       | NA    |                     |          |          |                   |
| NA       | NA    |                     |          |          |                   |
| NA       | NA    |                     |          |          |                   |
| NA       | NA    |                     |          |          |                   |
| NA       | NA    |                     |          |          |                   |

Bo = 4064 ppm\*\*  
Yc = 27.3\*\*

\* corresponds to data extracted from Table 6 on page 33.  
\*\*estimated from available MLSS measurements.

-----

Substrate : 2-chlorophenol  
Culture : m1ss (unacclimated sludge)  
Condition : 23C & pH 8.0-8.1

Substrate : 2-chlorophenol  
Culture : m1ss (unacclimated sludge)  
Condition : 23C & pH 8.0-8.1

E-103

\* corresponds to data extracted from Table 6 on page 33.



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Culture : miss

Condition : 22C

E-104

\* corresponds to data extracted from Table 1 on page 31.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Variable Biomass

Data source -- Pak Thesis (data set #9)\*; Substrate : phenol  
Culture : mlsa  
Condition : 22C & pH 7.5-7.8

Num.pts.= 10

| Raw Data |       | Summary of results: |          |          |                   |
|----------|-------|---------------------|----------|----------|-------------------|
| S(ppm)   | t(hr) | Kinetic Model       | ko       | K        | avg dt^2 avg dS^2 |
| 99.09    | 0     | Zero-order          |          |          |                   |
| 96.76    | 1     | (1-parameter)       | 0.001025 | ---      | 0.440784 7.136757 |
| 94.48    | 2     | First-order         |          |          |                   |
| 91.48    | 3     | (1-parameter)       | 0.000027 | ---      | 5.956465 290.4399 |
| 86.22    | 4     | Monod Kinetics      |          |          |                   |
| 82.67    | 5     | (2-parameter)       | 0.000906 | -4.47746 | 0.362396 ERR      |
| 76.66    | 6     |                     |          |          |                   |
| 67.93    | 7.42  |                     |          |          |                   |
| 10.66    | 22.75 |                     |          |          |                   |
| 7.54     | 24    |                     |          |          |                   |
| NA       | NA    |                     |          |          |                   |
| NA       | NA    |                     |          |          |                   |
| NA       | NA    |                     |          |          |                   |
| NA       | NA    |                     |          |          |                   |
| NA       | NA    |                     |          |          |                   |
| NA       | NA    |                     |          |          |                   |
| NA       | NA    |                     |          |          |                   |
| NA       | NA    |                     |          |          |                   |
| NA       | NA    |                     |          |          |                   |
| NA       | NA    |                     |          |          |                   |
| NA       | NA    |                     |          |          |                   |
| NA       | NA    |                     |          |          |                   |
| NA       | NA    |                     |          |          |                   |
| NA       | NA    |                     |          |          |                   |
| NA       | NA    |                     |          |          |                   |

Bo = 4026 ppm \*\* \* corresponds to data extracted from Table 1 on page 31.  
Yc = -6.6 \*\* \*\*estimated from available MLSS measurements.

.....

Substrate : phenol  
Culture : mls  
Condition : 21C & pH 7.5-7.8

Num.pts.= 8

[illegible]

\* corresponds to data extracted from Table 2 on page 31.

|   |   |   |   |   |   |   |   |   |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |   |
|---|---|---|---|---|---|---|---|---|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|---|
| 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 | 27 | 28 | 29 | 30 | 31 | 32 | 33 | 34 | 35 | 36 | 37 | 38 | 39 | 40 | 41 | 42 | 43 | 44 | 45 | 46 | 47 | 48 | 49 | 50 | 51 | 52 | 53 | 54 | 55 | 56 | 57 | 58 | 59 | 60 | 61 | 62 | 63 | 64 | 65 | 66 | 67 | 68 | 69 | 70 | 71 | 72 | 73 | 74 | 75 | 76 | 77 | 78 | 79 | 80 | 81 | 82 | 83 | 84 | 85 | 86 | 87 | 88 | 89 | 90 | 91 | 92 | 93 | 94 | 95 | 96 | 97 | 98 | 99 | 100 | 101 | 102 | 103 | 104 | 105 | 106 | 107 | 108 | 109 | 110 | 111 | 112 | 113 | 114 | 115 | 116 | 117 | 118 | 119 | 120 | 121 | 122 | 123 | 124 | 125 | 126 | 127 | 128 | 129 | 130 | 131 | 132 | 133 | 134 | 135 | 136 | 137 | 138 | 139 | 140 | 141 | 142 | 143 | 144 | 145 | 146 | 147 | 148 | 149 | 150 | 151 | 152 | 153 | 154 | 155 | 156 | 157 | 158 | 159 | 160 | 161 | 162 | 163 | 164 | 165 | 166 | 167 | 168 | 169 | 170 | 171 | 172 | 173 | 174 | 175 | 176 | 177 | 178 | 179 | 180 | 181 | 182 | 183 | 184 | 185 | 186 | 187 | 188 | 189 | 190 | 191 | 192 | 193 | 194 | 195 | 196 | 197 | 198 | 199 | 200 | 201 | 202 | 203 | 204 | 205 | 206 | 207 | 208 | 209 | 210 | 211 | 212 | 213 | 214 | 215 | 216 | 217 | 218 | 219 | 220 | 221 | 222 | 223 | 224 | 225 | 226 | 227 | 228 | 229 | 230 | 231 | 232 | 233 | 234 | 235 | 236 | 237 | 238 | 239 | 240 | 241 | 242 | 243 | 244 | 245 | 246 | 247 | 248 | 249 | 250 | 251 | 252 | 253 | 254 | 255 | 256 | 257 | 258 | 259 | 260 | 261 | 262 | 263 | 264 | 265 | 266 | 267 | 268 | 269 | 270 | 271 | 272 | 273 | 274 | 275 | 276 | 277 | 278 | 279 | 280 | 281 | 282 | 283 | 284 | 285 | 286 | 287 | 288 | 289 | 290 | 291 | 292 | 293 | 294 | 295 | 296 | 297 | 298 | 299 | 300 | 301 | 302 | 303 | 304 | 305 | 306 | 307 | 308 | 309 | 310 | 311 | 312 | 313 | 314 | 315 | 316 | 317 | 318 | 319 | 320 | 321 | 322 | 323 | 324 | 325 | 326 | 327 | 328 | 329 | 330 | 331 | 332 | 333 | 334 | 335 | 336 | 337 | 338 | 339 | 340 | 341 | 342 | 343 | 344 | 345 | 346 | 347 | 348 | 349 | 350 | 351 | 352 | 353 | 354 | 355 | 356 | 357 | 358 | 359 | 360 | 361 | 362 | 363 | 364 | 365 | 366 | 367 | 368 | 369 | 370 | 371 | 372 | 373 | 374 | 375 | 376 | 377 | 378 | 379 | 380 | 381 | 382 | 383 | 384 | 385 | 386 | 387 | 388 | 389 | 390 | 391 | 392 | 393 | 394 | 395 | 396 | 397 | 398 | 399 | 400 | 401 | 402 | 403 | 404 | 405 | 406 | 407 | 408 | 409 | 410 | 411 | 412 | 413 | 414 | 415 | 416 | 417 | 418 | 419 | 420 | 421 | 422 | 423 | 424 | 425 | 426 | 427 | 428 | 429 | 430 | 431 | 432 | 433 | 434 | 435 | 436 | 437 | 438 | 439 | 440 | 441 | 442 | 443 | 444 | 445 | 446 | 447 | 448 | 449 | 450 | 451 | 452 | 453 | 454 | 455 | 456 | 457 | 458 | 459 | 460 | 461 | 462 | 463 | 464 | 465 | 466 | 467 | 468 | 469 | 470 | 471 | 472 | 473 | 474 | 475 | 476 | 477 | 478 | 479 | 480 | 481 | 482 | 483 | 484 | 485 | 486 | 487 | 488 | 489 | 490 | 491 | 492 | 493 | 494 | 495 | 496 | 497 | 498 | 499 | 500 | 501 | 502 | 503 | 504 | 505 | 506 | 507 | 508 | 509 | 510 | 511 | 512 | 513 | 514 | 515 | 516 | 517 | 518 | 519 | 520 | 521 | 522 | 523 | 524 | 5 |
|---|---|---|---|---|---|---|---|---|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|---|

Substrate : 2,4-dichlorophenol  
Culture : mlss  
Condition : 23C & pH 7.4-7.5

Condition : 23C & pH 7.4-7.5

E-107

\*corresponds to data extracted from Table 35 on page 82.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Variable Biomass  
-----

Data source -- Salerno Thesis (data set #1)\*;

Substrate : 2,4-dichlorophenol  
Culture : mlss  
Condition : 23C & pH 7.4-7.5

Num.pts.= 6

| Raw Data |       | Summary of results: |           |          |          |          |
|----------|-------|---------------------|-----------|----------|----------|----------|
| S(ppm)   | t(hr) | Kinetic Model       | ko        | K        | avg dt^2 | avg dS^2 |
| 11.5     | 0     | Zero-order          |           |          |          |          |
| 11.1     | 90    | (1-parameter)       | 0.000061  | ---      | 2249.527 | 0.235119 |
| 8.8      | 180   | First-order         |           |          |          |          |
| 8.3      | 280   | (1-parameter)       | 0.000006  | ---      | 1887.759 | 0.188466 |
| 8.2      | 365   | Monod Kinetics      |           |          |          |          |
| 7.2      | 455   | (2-parameter)       | -0.000005 | -17.5957 | 1735.872 | 0.190494 |
| NA       | NA    |                     |           |          |          |          |
| NA       | NA    |                     |           |          |          |          |
| NA       | NA    |                     |           |          |          |          |
| NA       | NA    |                     |           |          |          |          |
| NA       | NA    |                     |           |          |          |          |
| NA       | NA    |                     |           |          |          |          |
| NA       | NA    |                     |           |          |          |          |
| NA       | NA    |                     |           |          |          |          |
| NA       | NA    |                     |           |          |          |          |
| NA       | NA    |                     |           |          |          |          |
| NA       | NA    |                     |           |          |          |          |
| NA       | NA    |                     |           |          |          |          |
| NA       | NA    |                     |           |          |          |          |
| NA       | NA    |                     |           |          |          |          |
| NA       | NA    |                     |           |          |          |          |
| NA       | NA    |                     |           |          |          |          |
| NA       | NA    |                     |           |          |          |          |
| NA       | NA    |                     |           |          |          |          |
| NA       | NA    |                     |           |          |          |          |
| NA       | NA    |                     |           |          |          |          |

Bo = 169 ppm\*\*  
Yc = -1.45 \*\*

\* corresponds to data extracted from Table 35 on page 82.  
\*\*estimated from available MLSS measurements.

Appendix F

Compilation of Analysis Results from the Study  
of the Effect of Experimental Error in Biodegradation  
Data on Kinetic Model Selection

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Tabulation of Ideal S vs. t Data  
(Constant-Biomass Behavior Assumed)\*

| <u>S(ppm)</u> | <u>t(hr)</u> | <u>S(ppm)</u> | <u>t(hr)</u> | <u>S(ppm)</u> | <u>t(hr)</u> | <u>S(ppm)</u> | <u>t(hr)</u> | <u>S(ppm)</u> | <u>t(hr)</u> |
|---------------|--------------|---------------|--------------|---------------|--------------|---------------|--------------|---------------|--------------|
| 100.00        | 0            | 65.05         | 149.40       | 33.61         | 298.80       | 10.25         | 448.20       | 1.23          | 597.60       |
| 98.20         | 7.47         | 63.37         | 156.87       | 32.20         | 306.27       | 9.44          | 455.67       | 1.08          | 605.07       |
| 96.41         | 14.94        | 61.70         | 164.34       | 30.80         | 313.74       | 8.67          | 463.14       | 0.95          | 612.54       |
| 94.62         | 22.41        | 60.04         | 171.81       | 29.42         | 321.21       | 7.94          | 470.61       | 0.84          | 620.01       |
| 92.83         | 29.88        | 58.39         | 179.28       | 28.07         | 328.68       | 7.21          | 478.08       | 0.74          | 627.48       |
| 91.05         | 37.35        | 56.75         | 186.75       | 26.73         | 336.15       | 6.60          | 485.55       | 0.65          | 634.95       |
| 89.28         | 44.82        | 55.12         | 194.22       | 25.43         | 343.62       | 6.00          | 493.02       | 0.57          | 642.42       |
| 87.51         | 52.29        | 53.50         | 201.69       | 24.14         | 351.09       | 5.43          | 500.49       | 0.50          | 649.89       |
| 85.74         | 59.76        | 51.89         | 209.16       | 22.88         | 358.56       | 4.98          | 507.96       | 0.44          | 657.36       |
| 83.98         | 67.23        | 50.29         | 216.63       | 21.65         | 366.03       | 4.42          | 515.43       | 0.38          | 664.83       |
| 82.23         | 74.70        | 48.71         | 224.10       | 20.45         | 373.50       | 3.98          | 522.90       | 0.34          | 672.30       |
| 80.48         | 82.17        | 47.13         | 231.57       | 19.28         | 380.97       | 3.57          | 530.37       | 0.29          | 679.77       |
| 78.74         | 89.64        | 45.57         | 239.04       | 18.14         | 388.44       | 3.19          | 537.84       | 0.26          | 687.24       |
| 77.00         | 97.11        | 44.02         | 246.51       | 17.03         | 395.91       | 2.85          | 545.31       | 0.23          | 694.71       |
| 75.27         | 104.58       | 42.49         | 253.98       | 15.95         | 403.38       | 2.54          | 552.78       | 0.20          | 702.18       |
| 73.55         | 112.05       | 40.97         | 261.45       | 14.91         | 410.85       | 2.26          | 560.25       | 0.18          | 709.65       |
| 71.83         | 119.52       | 39.47         | 268.92       | 13.90         | 418.32       | 2.00          | 567.72       | 0.16          | 717.12       |
| 70.13         | 126.99       | 37.98         | 276.39       | 12.97         | 425.79       | 1.78          | 575.19       | 0.14          | 724.59       |
| 68.45         | 134.46       | 36.41         | 283.86       | 12.01         | 433.26       | 1.57          | 582.66       | 0.12          | 732.06       |
| 66.73         | 141.93       | 35.05         | 291.33       | 11.10         | 440.73       | 1.39          | 590.13       | 0.10          | 739.53       |

-----  
 \* Refer to Figure 104: data derived using the M2 model with  $k = 0.278$  ppm/hr.,  
 $K = 15.3$  ppm and  $S_0 = 100$  ppm!



Tabulation of Ideal S vs. t Data  
(Variable-Biomass Behavior Assumed)\*

| <u>S(ppm)</u> | <u>t(hr)</u> | <u>S(ppm)</u> | <u>t(hr)</u> | <u>S(ppm)</u> | <u>t(hr)</u> | <u>S(ppm)</u> | <u>t(hr)</u> | <u>S(ppm)</u> | <u>t(hr)</u> |
|---------------|--------------|---------------|--------------|---------------|--------------|---------------|--------------|---------------|--------------|
| 100.00        | 0            | 96.97         | 7.336        | 88.83         | 14.672       | 67.71         | 22.008       | 21.77         | 29.344       |
| 99.91         | 0.367        | 96.73         | 7.703        | 88.18         | 15.039       | 66.07         | 22.375       | 19.09         | 29.711       |
| 99.81         | 0.734        | 96.47         | 8.070        | 87.50         | 15.406       | 64.36         | 22.742       | 16.50         | 30.078       |
| 99.71         | 1.100        | 96.20         | 8.436        | 86.78         | 15.772       | 62.50         | 23.108       | 14.03         | 30.444       |
| 99.61         | 1.467        | 95.91         | 8.803        | 86.03         | 16.139       | 60.73         | 23.475       | 11.70         | 30.811       |
| 99.50         | 1.834        | 95.62         | 9.170        | 85.23         | 16.506       | 58.80         | 23.842       | 9.56          | 31.178       |
| 99.38         | 2.201        | 95.30         | 9.537        | 84.41         | 16.873       | 56.79         | 24.209       | 7.64          | 31.545       |
| 99.26         | 2.568        | 94.97         | 9.904        | 83.54         | 17.240       | 54.77         | 24.576       | 5.98          | 31.912       |
| 99.13         | 2.934        | 94.63         | 10.270       | 82.63         | 17.606       | 52.55         | 24.942       | 4.57          | 32.278       |
| 99.00         | 3.301        | 94.26         | 10.637       | 81.67         | 17.973       | 50.31         | 25.309       | 3.42          | 32.645       |
| 98.86         | 3.668        | 93.88         | 11.004       | 80.67         | 18.340       | 48.00         | 25.676       | 2.51          | 33.012       |
| 98.71         | 4.035        | 93.48         | 11.371       | 79.62         | 18.707       | 45.61         | 26.043       | 1.81          | 33.379       |
| 98.55         | 4.402        | 93.06         | 11.738       | 78.52         | 19.074       | 43.15         | 26.410       | 1.29          | 33.746       |
| 98.39         | 4.768        | 92.62         | 12.104       | 77.38         | 19.440       | 40.63         | 26.776       | 0.91          | 34.112       |
| 98.21         | 5.135        | 92.15         | 12.471       | 76.17         | 19.807       | 38.03         | 27.143       | 0.64          | 34.479       |
| 98.03         | 5.502        | 91.53         | 12.838       | 74.91         | 20.174       | 35.39         | 27.510       | 0.44          | 34.846       |
| 97.82         | 5.869        | 91.15         | 13.205       | 73.60         | 20.541       | 32.70         | 27.877       | 0.31          | 35.213       |
| 97.64         | 6.236        | 90.61         | 13.572       | 72.22         | 20.908       | 29.97         | 28.244       | 0.21          | 35.580       |
| 97.43         | 6.602        | 90.05         | 13.938       | 70.78         | 21.274       | 27.23         | 28.610       | 0.15          | 35.946       |
| 97.21         | 6.969        | 89.46         | 14.305       | 69.28         | 21.641       | 24.49         | 28.977       | 0.10          | 36.313       |

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 \* Refer to Figure 104; data derived using MV model with  $k_o = 0.278$  ppm/ppm-hr..  
 $K = 15.3$  ppm,  $Y_c = 0.568$  ppm/ppm,  $B_o = 1$  ppm and  $S_o = 100$  ppm!

Tabulation of 100 Randomly-Generated Numbers  
in the Range Between 0 and 1\*

|            |            |            |            |             |
|------------|------------|------------|------------|-------------|
| 1) 0.1624  | 21) 0.7856 | 41) 0.3498 | 61) 0.4246 | 81) 0.5535  |
| 2) 0.0325  | 22) 0.4182 | 42) 0.9690 | 62) 0.0112 | 82) 0.8565  |
| 3) 0.3598  | 23) 0.4727 | 43) 0.0549 | 63) 0.1628 | 83) 0.8851  |
| 4) 0.5767  | 24) 0.4989 | 44) 0.0016 | 64) 0.8920 | 84) 0.9978  |
| 5) 0.3652  | 25) 0.8508 | 45) 0.5949 | 65) 0.1524 | 85) 0.0871  |
| 6) 0.6704  | 26) 0.4570 | 46) 0.4918 | 66) 0.0744 | 86) 0.5135  |
| 7) 0.6956  | 27) 0.5819 | 47) 0.7358 | 67) 0.2578 | 87) 0.1750  |
| 8) 0.8096  | 28) 0.4119 | 48) 0.1760 | 68) 0.8828 | 88) 0.3688  |
| 9) 0.9215  | 29) 0.3318 | 49) 0.3151 | 69) 0.4117 | 89) 0.2176  |
| 10) 0.2596 | 30) 0.2722 | 50) 0.5892 | 70) 0.5194 | 90) 0.3684  |
| 11) 0.1653 | 31) 0.3740 | 51) 0.6810 | 71) 0.1486 | 91) 0.8479  |
| 12) 0.6528 | 32) 0.2642 | 52) 0.5926 | 72) 0.4391 | 92) 0.6139  |
| 13) 0.6354 | 33) 0.0298 | 53) 0.3088 | 73) 0.0332 | 93) 0.7609  |
| 14) 0.3759 | 34) 0.4244 | 54) 0.8427 | 74) 0.9246 | 94) 0.9966  |
| 15) 0.0775 | 35) 0.1783 | 55) 0.1934 | 75) 0.1821 | 95) 0.2126  |
| 16) 0.1685 | 36) 0.1036 | 56) 0.3077 | 76) 0.5909 | 96) 0.7720  |
| 17) 0.3201 | 37) 0.7668 | 57) 0.4067 | 77) 0.8094 | 97) 0.5183  |
| 18) 0.5683 | 38) 0.4717 | 58) 0.7954 | 78) 0.8540 | 98) 0.9589  |
| 19) 0.7379 | 39) 0.2975 | 59) 0.5844 | 79) 0.6551 | 99) 0.5748  |
| 20) 0.4278 | 40) 0.9983 | 60) 0.3868 | 80) 0.4240 | 100) 0.9259 |

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\* As generated on the IBM PC using the Basic program "Randomize."

Tabulation of u Values for the Corresponding  
100 Randomly-Generated P(u) Values from Page F-5\*

|               |               |               |               |               |
|---------------|---------------|---------------|---------------|---------------|
| 1) -0.985 u'  | 21) 0.790 u'  | 41) -0.385 u' | 61) -0.190 u' | 81) 0.135 u'  |
| 2) -1.845 u'  | 22) -0.205 u' | 42) 1.865 u'  | 62) -2.280 u' | 82) 1.065 u'  |
| 3) -0.360 u'  | 23) -0.070 u' | 43) -1.600 u' | 63) -0.985 u' | 83) 1.200 u'  |
| 4) 0.190 u'   | 24) 0.000 u'  | 44) -2.950 u' | 64) 1.240 u'  | 84) 2.850 u'  |
| 5) -0.345 u'  | 25) 1.040 u'  | 45) 0.240 u'  | 65) -1.025 u' | 85) -1.360 u' |
| 6) 0.440 u'   | 26) -0.110 u' | 46) -0.020 u' | 66) -1.445 u' | 86) 0.035 u'  |
| 7) 0.510 u'   | 27) 0.205 u'  | 47) 0.630 u'  | 67) -0.650 u' | 87) -0.935 u' |
| 8) 0.880 u'   | 28) -0.220 u' | 48) -0.930 u' | 68) 1.190 u'  | 88) -0.335 u' |
| 9) 1.415 u'   | 29) -0.435 u' | 49) -0.480 u' | 69) -0.225 u' | 89) -0.780 u' |
| 10) -0.645 u' | 30) -0.610 u' | 50) 0.225 u'  | 70) 0.050 u'  | 90) -0.335 u' |
| 11) -0.970 u' | 31) -0.320 u' | 51) 0.470 u'  | 71) -1.040 u' | 91) 1.030 u'  |
| 12) 0.390 u'  | 32) -0.630 u' | 52) 0.235 u'  | 72) -0.155 u' | 92) 0.290 u'  |
| 13) 0.345 u'  | 33) -1.890 u' | 53) -0.500 u' | 73) -1.835 u' | 93) 0.710 u'  |
| 14) -0.320 u' | 34) -0.190 u' | 54) 1.005 u'  | 74) 1.440 u'  | 94) 2.710 u'  |
| 15) -1.420 u' | 35) -0.920 u' | 55) -0.865 u' | 75) -0.910 u' | 95) -0.800 u' |
| 16) -0.960 u' | 36) -1.260 u' | 56) -0.500 u' | 76) 0.230 u'  | 96) 0.745 u'  |
| 17) -0.470 u' | 37) 0.730 u'  | 57) -0.235 u' | 77) 0.880 u'  | 97) 0.045 u'  |
| 18) 0.170 u'  | 38) -0.070 u' | 58) 0.825 u'  | 78) 1.055 u'  | 98) 1.740 u'  |
| 19) 0.640 u'  | 39) -0.530 u' | 59) 0.210 u'  | 79) 0.400 u'  | 99) 0.190 u'  |
| 20) -0.180 u' | 40) 2.930 u'  | 60) -0.285 u' | 80) -0.190 u' | 100) 1.445 u' |

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\* u, P(u) and u' are defined in Equation (5) on page 154!

Effect of Total Number of Data Points on Regression Results (for  $u' = 0$ )\*

Case 1: Ideal S vs. t data from page F-3 for constant-biomass behavior (as determined from the M2 model:  $-dS/dt = 0.278 S/(15.3 + S)$ )

Experiment A: 100 points from 100 ppm to 0.1 ppm equally spaced with respect to time.

| <u>Model</u> | <u>ko(ppm/ppm-hr)</u> | <u>K(ppm)</u> | <u>Avg(t-tcalc)^2</u> |
|--------------|-----------------------|---------------|-----------------------|
| 1) M3        | 0.2789                | 15.44         | 0.272                 |
| 2) M2        | 0.2786                | 15.42         | 0.279                 |
| 3) MV        | -0.0532               | -262.37       | 1542                  |
| 4) FV        | 0.000256              | -             | 2569                  |
| 5) Z2        | 0.1536                | -             | 3934                  |
| 6) F2        | 0.009811              | -             | 4052                  |
| 7) Z1        | 0.1778                | -             | 4895                  |
| 8) F1        | 0.007351              | -             | 12582                 |
| 9) ZV        | 0.01568               | -             | 22911                 |

Percent error in rate constants for M2 and M3:\*\*

|    | <u>ko</u> | <u>K</u> |
|----|-----------|----------|
| M2 | +0.21%    | +0.77%   |
| M3 | +0.32%    | +0.94%   |

Experiment B: 34 points from 100 ppm to 0.1 ppm equally spaced with respect to time.

| <u>Model</u> | <u>ko(ppm/ppm-hr)</u> | <u>K(ppm)</u> | <u>Avg(t-tcalc)^2</u> |
|--------------|-----------------------|---------------|-----------------------|
| 1) M3        | 0.2788                | 15.43         | 0.284                 |
| 2) M2        | 0.2785                | 15.41         | 0.289                 |
| 3) MV        | -0.0554               | -270.37       | 1545                  |
| 4) FV        | 0.000256              | -             | 2509                  |
| 5) Z2        | 0.1535                | -             | 4182                  |
| 6) F2        | 0.009850              | -             | 4278                  |
| 7) Z1        | 0.1768                | -             | 5118                  |
| 8) F1        | 0.007432              | -             | 12735                 |
| 9) ZV        | 0.01555               | -             | 23242                 |

Percent error in rate constants for M2 and M3:\*\*

|    | <u>ko</u> | <u>K</u> |
|----|-----------|----------|
| M2 | +0.18%    | +0.70%   |
| M3 | +0.27%    | +0.83%   |

\* No experimental error was assumed to be present.

\*\* Percent error = ((regressed value - "real" value)/("real" value))\*100%

Experiment C: 12 points from 100 ppm to 0.1 ppm equally spaced with respect to time.

| <u>Model</u> | <u>ko(ppm/ppm-hr)</u> | <u>K(ppm)</u> | <u>Avg(t-tcalc)^2</u> |
|--------------|-----------------------|---------------|-----------------------|
| 1) M3        | 0.2781                | 15.33         | 0.0577                |
| 2) M2        | 0.2781                | 15.33         | 0.0580                |
| 3) MV        | -0.0642               | -303.72       | 1484                  |
| 4) FV        | 0.000256              | -             | 2233                  |
| 5) Z2        | 0.1534                | -             | 4916                  |
| 6) F2        | 0.009968              | -             | 4957                  |
| 7) Z1        | 0.1739                | -             | 5772                  |
| 8) F1        | 0.007672              | -             | 13147                 |
| 9) ZV        | 0.01515               | -             | 23844                 |

Percent error in rate constants for M2 and M3:

|    | <u>ko</u> | <u>K</u> |
|----|-----------|----------|
| M2 | +0.03%    | +0.16%   |
| M3 | +0.05%    | +0.19%   |

Experiment D: 10 points from 100 ppm to 0.1 ppm equally spaced with respect to time.

| <u>Model</u> | <u>ko(ppm/ppm-hr)</u> | <u>K(ppm)</u> | <u>Avg(t-tcalc)^2</u> |
|--------------|-----------------------|---------------|-----------------------|
| 1) M3        | 0.2780                | 15.31         | 0.0228                |
| 2) M2        | 0.2780                | 15.31         | 0.0229                |
| 3) MV        | -0.06780              | -316.76       | 1442                  |
| 4) FV        | 0.000256              | -             | 2120                  |
| 5) Z2        | 0.1533                | -             | 5156                  |
| 6) F2        | 0.009998              | -             | 5173                  |
| 7) Z1        | 0.1730                | -             | 5984                  |
| 8) F1        | 0.007745              | -             | 13242                 |
| 9) ZV        | 0.01501               | -             | 23926                 |

Percent error in rate constants for M2 and M3:

|    | <u>ko</u> | <u>K</u> |
|----|-----------|----------|
| M2 | +0.01%    | +0.08%   |
| M3 | +0.01%    | +0.06%   |

Experiment E: 4 points from 100 ppm to 0.1 ppm equally spaced with respect to time.

| <u>Model</u> | <u>ko(ppm/ppm-hr)</u> | <u>K(ppm)</u> | <u>Avg(t-tcalc)^2</u> |
|--------------|-----------------------|---------------|-----------------------|
| 1) M3        | 0.2780                | 15.30         | 0.000440              |
| 2) M2        | 0.2780                | 15.30         | 0.000478              |
| 3) MV        | -0.1847               | -769.87       | 681                   |
| 4) FV        | 0.000255              | -             | 772                   |
| 5) F2        | 0.0102                | -             | 7250                  |
| 6) Z2        | 0.1523                | -             | 7632                  |
| 7) Z1        | 0.1638                | -             | 8104                  |
| 8) F1        | 0.008406              | -             | 13500                 |
| 9) ZV        | 0.01347               | -             | 22169                 |

Percent error in rate constants for M2 and M3:

|    | <u>ko</u> | <u>K</u> |
|----|-----------|----------|
| M2 | -0.01%    | -0.02%   |
| M3 | -0.02%    | -0.02%   |

Case 2: Ideal S vs. t data from page F-4 for variable-biomass behavior (as determined from the MV model:  $-dS/dt = 0.278 (1 + 0.568(100-S))S/(15.3 + S)$ )

Experiment A: 100 points from 100 ppm to 0.1 ppm equally spaced with respect to time:

| <u>Model</u> | <u>ko(ppm/ppm-hr)</u> | <u>K(ppm)</u> | <u>Avg(t-tcalc)^2</u> |
|--------------|-----------------------|---------------|-----------------------|
| 1) MV        | 0.2781                | 15.60         | 0.000133              |
| 2) ZV        | 0.2257                | -             | 1.583                 |
| 3) M3        | 2.979                 | -4.020        | 11.80                 |
| 4) Z2        | 3.545                 | -             | 13.06                 |
| 5) FV        | 0.003630              | -             | 26.62                 |
| 6) M2        | 1.930                 | -6.630        | 39.97                 |
| 7) F2        | 0.2036                | -             | 48.17                 |
| 8) Z1        | 2.493                 | -             | 49.04                 |
| 9) F1        | 0.1172                | -             | 179.9                 |

Percent error in rate constants for MV:

% error in ko = +0.04%

% error in K = +1.99%

Experiment B: 34 points from 100 ppm to 0.1 ppm equally spaced with respect to time.

| <u>Model</u> | <u>ko(ppm/ppm-hr)</u> | <u>K(ppm)</u> | <u>Avg(t-tcalc)^2</u> |
|--------------|-----------------------|---------------|-----------------------|
| 1) MV        | 0.2781                | 15.60         | 0.000024              |
| 2) ZV        | 0.2249                | -             | 1.782                 |
| 3) M3        | 2.998                 | -3.561        | 12.39                 |
| 4) Z2        | 3.516                 | -             | 13.51                 |
| 5) FV        | 0.003706              | -             | 28.71                 |
| 6) M2        | 1.967                 | -6.020        | 39.88                 |
| 7) Z1        | 2.502                 | -             | 48.19                 |
| 8) F2        | 0.2120                | -             | 50.27                 |
| 9) F1        | 0.1234                | -             | 181.5                 |

Percent error in rate constants for MV:

% error in ko = +0.03%

% error in K = +1.94%

Experiment C: 12 points from 100 ppm to 0.1 ppm equally spaced with respect to time.

| <u>Model</u> | <u>ko(ppm/ppm-hr)</u> | <u>K(ppm)</u> | <u>Avg(t-tcalc)^2</u> |
|--------------|-----------------------|---------------|-----------------------|
| 1) MV        | 0.2781                | 15.60         | 0.000024              |
| 2) ZV        | 0.2226                | -             | 2.399                 |
| 3) M3        | 3.009                 | -2.656        | 13.93                 |
| 4) Z2        | 3.431                 | -             | 14.81                 |
| 5) FV        | 0.003925              | -             | 35.61                 |
| 6) M2        | 2.044                 | -4.745        | 38.99                 |
| 7) Z1        | 2.521                 | -             | 45.67                 |
| 8) F2        | 0.2331                | -             | 55.71                 |
| 9) F1        | 0.1400                | -             | 183.0                 |

Percent error in rate constants for MV:

% error in ko = +0.04%  
 % error in K = +1.95%

Experiment D: 10 points from 100 ppm to 0.1 ppm equally spaced with respect to time.

| <u>Model</u> | <u>ko(ppm/ppm-hr)</u> | <u>K(ppm)</u> | <u>Avg(t-tcalc)^2</u> |
|--------------|-----------------------|---------------|-----------------------|
| 1) MV        | 0.2780                | 15.57         | 0.000008              |
| 2) ZV        | 0.2218                | -             | 2.600                 |
| 3) M3        | 3.013                 | -2.409        | 14.49                 |
| 4) Z2        | 3.406                 | -             | 15.28                 |
| 5) FV        | 0.003994              | -             | 35.61                 |
| 6) M2        | 2.068                 | -4.403        | 38.84                 |
| 7) Z1        | 2.527                 | -             | 45.01                 |
| 8) F2        | 0.2389                | -             | 57.36                 |
| 9) F1        | 0.1450                | -             | 182.8                 |

Percent error in rate constants for MV:

% error in ko = +0.002%  
 % error in K = +1.79%



Experiment E: 4 points from 100 ppm to 0.1 ppm equally spaced with respect to time.

| <u>Model</u> | <u>ko(ppm/ppm-hr)</u> | <u>K(ppm)</u> | <u>Avg(t-tcalc)^2</u> |
|--------------|-----------------------|---------------|-----------------------|
| 1) MV        | 0.278001              | 15.57         | 0.000002              |
| 2) ZV        | 0.2126                | -             | 4.168                 |
| 3) M3        | 1.886                 | -5.589        | 9.113                 |
| 4) M2        | 1.549                 | -6.323        | 15.12                 |
| 5) Z2        | 3.073                 | -             | 17.93                 |
| 6) Z1        | 2.499                 | -             | 36.25                 |
| 7) FV        | 0.004659              | -             | 38.35                 |
| 8) F2        | 0.2632                | -             | 61.21                 |
| 9) F1        | 0.1810                | -             | 146.1                 |

Percent error in rate constants for MV:

% error in ko = +0.0004%  
 % error in K = +1.79%

Effect of Random Experimental Error in S on Regression Results

Case 1: Ideal S vs. t data from page F-3 for constant-biomass behavior modified to include random error in experimental measurements using page F-6.\*

Experiment A:  $u' = 0.1$  ppm\*\*

| <u>Model</u> | <u>ko(ppm/ppm-hr)</u> | <u>K(ppm)</u> | <u>Avg(t-tcalc)^2</u> |
|--------------|-----------------------|---------------|-----------------------|
| 1) M3        | 0.2939                | 17.95         | 169.3                 |
| 2) M2        | 0.2891                | 17.52         | 171.2                 |

Percent error in rate constants for M2 and M3:

|    | <u>ko</u> | <u>K</u> |
|----|-----------|----------|
| M2 | +3.99%    | +14.51%  |
| M3 | +5.72%    | +17.33%  |

Experiment B:  $u' = 0.25$  ppm\*\*

| <u>Model</u> | <u>ko(ppm/ppm-hr)</u> | <u>K(ppm)</u> | <u>Avg(t-tcalc)^2</u> |
|--------------|-----------------------|---------------|-----------------------|
| 1) M3        | 0.2830                | 16.72         | 759.1                 |
| 2) M2        | 0.2816                | 16.70         | 759.1                 |

Percent error in rate constants for M2 and M3:

|    | <u>ko</u> | <u>K</u> |
|----|-----------|----------|
| M2 | +1.29%    | + 9.15%  |
| M3 | +1.80%    | + 9.28%  |

\* 10 equally-spaced (with respect to time) S vs. t data points for the range of S from 100 ppm down to 0.1 ppm were used; variable-biomass models are inappropriate for this case and were not evaluated here.

\*\* The other constant-biomass models are poor (performing analogously to the case in which  $u' = 0$  on page F-8) and are not shown here.

Experiment C:  $u' = 0.5$  ppm

| <u>Model</u> | <u>ko(ppm/ppm-hr)</u> | <u>K(ppm)</u> | <u>Avg(t-tcalc)^2</u> |
|--------------|-----------------------|---------------|-----------------------|
| 1) M3        | 0.2220                | 8.518         | 2326                  |
| 2) M2        | 0.2368                | 9.521         | 2384                  |
| 3) Z2        | 0.1530                | -             | 5276                  |
| 4) Z1        | 0.1719                | -             | 6051                  |
| 5) F2        | 0.01094               | -             | 11362                 |
| 6) F1        | 0.008025              | -             | 22759                 |

Percent error in rate constants for M2 and M3:

|    | <u>ko</u> | <u>K</u> |
|----|-----------|----------|
| M2 | -14.8%    | -37.8%   |
| M3 | -20.2%    | -44.3%   |

Experiment D:  $u' = 1.0$  ppm\*

| <u>Model</u> | <u>ko(ppm/ppm-hr)</u> | <u>K(ppm)</u> | <u>Avg(t-tcalc)^2</u> |
|--------------|-----------------------|---------------|-----------------------|
| 1) M3        | 0.190717              | 4.493952      | 3604                  |
| 2) M2        | 0.208567              | 5.356304      | 3782                  |
| 3) Z2        | 0.152568              | -             | 5439                  |
| 4) Z1        | 0.170667              | -             | 6160                  |
| 5) F2        | 0.013728              | -             | 18951                 |
| 6) F1        | 0.009166              | -             | 38551                 |

Percent error in rate constants for M2 and M3:

|    | <u>ko</u> | <u>K</u> |
|----|-----------|----------|
| M2 | -25.0%    | -65.0%   |
| M3 | -31.4%    | -70.6%   |

\* Since the value of S at  $t = 657$  hr (upon adding the correction for experimental error) was negative and use of  $S = 0$  yields erroneous regression results for the first-order and Monod models because of the  $\ln$  terms present, its value was arbitrarily assumed to be 0.01 ppm for calculations sake.

Experiment E:  $u' = 2.0 \text{ ppm}^*$ 

| <u>Model</u> | <u>ko(ppm/ppm-hr)</u> | <u>K(ppm)</u> | <u>Avg(t-tcalc)^2</u> |
|--------------|-----------------------|---------------|-----------------------|
| 1) M3        | 0.181479              | 3.626129      | 4466                  |
| 2) M2        | 0.198053              | 4.365422      | 4660                  |
| 3) Z2        | 0.151813              | -             | 5801                  |
| 4) Z1        | 0.168296              | -             | 6414                  |
| 5) F2        | 0.014072              | -             | 21941                 |
| 6) F1        | 0.009092              | -             | 44232                 |

Percent error in rate constants for M2 and M3:

|    | <u>ko</u> | <u>K</u> |
|----|-----------|----------|
| M2 | -28.8%    | -71.5%   |
| M3 | -34.7%    | -76.3%   |

Experiment F:  $u' = 5.0 \text{ ppm}^*$ 

| <u>Model</u> | <u>ko(ppm/ppm-hr)</u> | <u>K(ppm)</u> | <u>Avg(t-tcalc)^2</u> |
|--------------|-----------------------|---------------|-----------------------|
| 1) M3        | 0.168382              | 2.258022      | 6523                  |
| 2) M2        | 0.178733              | 2.650142      | 6632                  |
| 3) Z2        | 0.150258              | -             | 7143                  |
| 4) Z1        | 0.161374              | -             | 7441                  |
| 5) F2        | 0.015080              | -             | 26972                 |
| 6) F1        | 0.009173              | -             | 54402                 |

Percent error in rate constants for M2 and M3:

|    | <u>ko</u> | <u>K</u> |
|----|-----------|----------|
| M2 | -35.7%    | -82.7%   |
| M3 | -39.4%    | -85.2%   |

\* Since the value of S at  $t = 657 \text{ hr}$  (upon adding the correction for experimental error) was negative and use of  $S = 0$  yields erroneous regression results for the first-order and Monod models because of the  $\ln$  terms present, its value was arbitrarily assumed to be  $0.1 \text{ ppm}$  for calculations sake.

Case 2: Ideal S vs. t data from page F-4 for variable-biomass behavior modified to include random error in experimental measurements using page F-6.\*

Experiment A:  $u' = 0.1$  ppm

| <u>Model</u> | <u>ko(ppm/ppm-hr)</u> | <u>K(ppm)</u> | <u>Avg(t-tcalc)^2</u> |
|--------------|-----------------------|---------------|-----------------------|
| 1) MV        | 0.2849                | 18.09         | 0.03121               |
| 2) ZV        | 0.2215                | -             | 2.549                 |
| 3) FV        | 0.003797              | -             | 27.70                 |

Percent error in rate constants for MV:

% error in ko = +2.48%  
 % error in K = +18.24%

Experiment B:  $u' = 0.25$  ppm

| <u>Model</u> | <u>ko(ppm/ppm-hr)</u> | <u>K(ppm)</u> | <u>Avg(t-tcalc)^2</u> |
|--------------|-----------------------|---------------|-----------------------|
| 1) MV        | 0.2897                | 20.04         | 0.1610                |
| 2) ZV        | 0.2210                | -             | 2.534                 |
| 3) FV        | 0.003663              | -             | 22.64                 |

Percent error in rate constants for MV:

% error in ko = +4.22%  
 % error in K = +30.95%

Experiment C:  $u' = 0.5$  ppm

| <u>Model</u> | <u>ko(ppm/ppm-hr)</u> | <u>K(ppm)</u> | <u>Avg(t-tcalc)^2</u> |
|--------------|-----------------------|---------------|-----------------------|
| 1) MV        | 0.2923                | 21.39         | 0.5758                |
| 2) ZV        | 0.2203                | -             | 2.717                 |
| 3) FV        | 0.003557              | -             | 15.43                 |

Percent error in rate constants for MV:

% error in ko = +5.15%  
 % error in K = +39.79%

\* 10 equally-spaced (with respect to time) S vs. t data points for the range of S from 100 ppm down to 0.1 ppm were used; constant-biomass models are poor (performing analogously to the case in which  $u' = 0$  on page F-11) and are not shown here.

Experiment D:  $u' = 1.0$  ppm

| <u>Model</u> | <u>ko(ppm/ppm-hr)</u> | <u>K(ppm)</u> | <u>Avg(t-tcalc)^2</u> |
|--------------|-----------------------|---------------|-----------------------|
| 1) MV        | 0.2927                | 22.16         | 2.531                 |
| 2) ZV        | 0.2194                | -             | 4.349                 |
| 3) FV        | 0.003464              | -             | 17.82                 |

Percent error in rate constants for MV:

% error in ko = +5.30%

% error in K = +44.85%

Experiment E:  $u' = 2.0$  ppm

| <u>Model</u> | <u>ko(ppm/ppm-hr)</u> | <u>K(ppm)</u> | <u>Avg(t-tcalc)^2</u> |
|--------------|-----------------------|---------------|-----------------------|
| 1) MV        | 0.4756                | 72.27         | 28.72                 |
| 2) FV        | 0.003496              | -             | 34.15                 |
| 3) ZV        | 0.2295                | -             | 35.32                 |

Percent error in rate constants for MV:

% error in ko = +71.07%

% error in K = +372.4%

Experiment F:  $u' = 5.0$  ppm\*

| <u>Model</u> | <u>ko(ppm/ppm-hr)</u> | <u>K(ppm)</u> | <u>Avg(t-tcalc)^2</u> |
|--------------|-----------------------|---------------|-----------------------|
| 1) MV        | N/A                   | N/A           | N/A                   |
| 2) ZV        | N/A                   | -             | N/A                   |
| 3) FV        | N/A                   | -             | N/A                   |

\* Regression results for this case are indeterminate because of negative values within ln functions (i.e.,  $B_0 + Y_{cSo} - Y_{cS}$  is negative for each variable-biomass model for the second point of the set, thereby making  $\ln(B_0 + Y_{cSo} - Y_{cS})$  indeterminate for that point and, hence, the entire set).

Effect of Total Number of Data Points on Regression Results for Case 1  
(Constant-Biomass Behavior Assumed) and  $u'$  Not equal to 0

Experiment A:  $u' = 1.0$  ppm

| <u>Number of Points*</u> | <u>M2 Model</u>                    |                     |                                  |
|--------------------------|------------------------------------|---------------------|----------------------------------|
|                          | <u>% Error in <math>k_o</math></u> | <u>% Error in K</u> | <u>Avg (t-tcalc)<sup>2</sup></u> |
| 100-4 = 96               | -3.9%                              | -1.4%               | 1307                             |
| 34-1 = 33                | -5.2%                              | -2.5%               | 1703                             |
| 12-0 = 12                | +9.9%                              | +53.1%              | 1972                             |
| 10-1 = 9                 | +87.9%                             | +156.0%             | 977                              |
| 4-0 = 4                  | +85.4%                             | +321.3%             | 1299                             |

Experiment B:  $u' = 5.0$  ppm

| <u>Number of Points*</u> | <u>M2 Model</u>                    |                     |                                  |
|--------------------------|------------------------------------|---------------------|----------------------------------|
|                          | <u>% Error in <math>k_o</math></u> | <u>% Error in K</u> | <u>Avg (t-tcalc)<sup>2</sup></u> |
| 100-11 = 89              | -13.7%                             | -7.2%               | 4010                             |
| 34-3 = 31                | -12.0%                             | +3.1%               | 3525                             |
| 12-1 = 11                | +93.2%                             | +515.7%             | 3216                             |
| 10-1 = 9                 | -24.6%                             | -37.9%              | 7128                             |
| 4-0 = 4                  | -49.8%                             | +119.2%             | 11985                            |

- \* Data points for which negative S values resulted, upon addition of random error terms, were excluded; this, in turn, has the effect of inflating the average S value in the latter portion of the set which otherwise would be obtained, thereby introducing a systematic error into the regression analysis results.

Effect of Data Spacing/Regularity on Regression Results\*

Case 1: Ideal S vs. t data from page F-3 for constant-biomass behavior modified to include random error in experimental measurements of magnitude  $u' = 1.0$  ppm using page F-6.

| <u>S vs. t Data Points Used**</u> | <u>M2 Model</u>                    |                     |                                  |
|-----------------------------------|------------------------------------|---------------------|----------------------------------|
|                                   | <u>% Error in <math>k_o</math></u> | <u>% Error in K</u> | <u>avg (t-tcalc)<sup>2</sup></u> |
| A) 1,2,3,4,5,6,7,8,9,100          | -10.4%                             | + 36.2%             | 4.1                              |
| B) 1,91,92,93,94,96,97,98,99,100  | -50.7%                             | -101.4%             | 465.5                            |
| C) 1,46,47,48,49,50,51,52,53,100  | +55.3%                             | +247.5%             | 34.4                             |
| D) 1,12,23,34,45,56,67,78,88,100  | -11.1%                             | - 19.9%             | 2636.3                           |
| E) 1,4,22,36,37,51,70,76,81,100   | +14.0%                             | + 64.5%             | 1533.8                           |

Case 2: Ideal S vs. t data from page F-4 for variable-biomass behavior modified to include random error in experimental measurements of magnitude  $u' = 1.0$  ppm using page F-6.

| <u>S vs. t Data Points Used**</u> | <u>M2 Model</u>                    |                     |                                  |
|-----------------------------------|------------------------------------|---------------------|----------------------------------|
|                                   | <u>% Error in <math>k_o</math></u> | <u>% Error in K</u> | <u>avg (t-tcalc)<sup>2</sup></u> |
| A) 1,2,3,4,5,6,7,8,9,100          | -150.7%                            | -658.1%             | 0.63182                          |
| B) 1,91,92,93,94,96,97,98,99,100  | - 11.1%                            | - 33.5%             | 0.67192                          |
| C) 1,46,47,48,49,50,51,52,53,100  | + 7.9%                             | + 73.4%             | 0.04231                          |
| D) 1,12,23,34,45,56,67,78,89,100  | + 2.5%                             | + 18.2%             | 0.03121                          |
| E) 1,4,22,36,37,51,70,76,81,100   | + 18.1%                            | +118.6%             | 4.22879                          |

\* 10 S vs. t data points of various spacings with respect to time evaluated in each case.

\*\* The numbers listed refer to the numerical sequence within each given data set that the S vs. t data points correspond to.



Effect of Data Range/Truncation on Regression Results (for  $u' = 1.0$  ppm)

Case 1: Ideal S vs. t data from page F-3 for constant-biomass behavior modified to include the corresponding random error correction terms from page F-6.\*

Experiment A: 100 ppm  $\rightarrow$  0.1 ppm (100 - 4 = 96 points)

|    | <u>Model</u> | <u>ko (ppm/ppm-hr)</u> | <u>K (ppm)</u> | <u>Avg (t-tcalc)<sup>2</sup></u> |
|----|--------------|------------------------|----------------|----------------------------------|
| 1) | M3           | 0.261042               | 14.51390       | 1303                             |
| 2) | M2           | 0.267129               | 15.08139       | 1307                             |
| 3) | Z2           | 0.156002               | -              | 4043                             |
| 4) | Z1           | 0.177875               | -              | 4801                             |
| 5) | F2           | 0.008775               | -              | 5574                             |
| 6) | F1           | 0.006609               | -              | 13006                            |

Percent error in rate constants for M2 and M3:

|    | <u>ko</u> | <u>K</u> |
|----|-----------|----------|
| M2 | -3.91%    | -1.43%   |
| M3 | -6.10%    | -5.14%   |

Experiment B: 100 ppm  $\rightarrow$  1.0 ppm (83-0 = 83 points)

|    | <u>Model</u> | <u>ko (ppm/ppm-hr)</u> | <u>K (ppm)</u> | <u>Avg (t-tcalc)<sup>2</sup></u> |
|----|--------------|------------------------|----------------|----------------------------------|
| 1) | M3           | 0.279558               | 15.70073       | 165                              |
| 2) | M2           | 0.273454               | 15.02311       | 167                              |
| 3) | Z2           | 0.176528               | -              | 1194                             |
| 4) | Z1           | 0.193365               | -              | 1488                             |
| 5) | F2           | 0.007495               | -              | 2590                             |
| 6) | F1           | 0.005781               | -              | 7021                             |

Percent error in rate constants for M2 and M3:

|    | <u>ko</u> | <u>K</u> |
|----|-----------|----------|
| M2 | -1.63%    | -1.81%   |
| M3 | +0.56%    | +2.62%   |

\* All points within the given S range which result in positive values of S (upon incorporating the random error terms) are included.

Experiment C: 100 ppm  $\rightarrow$  5.0 ppm (69 - 0 = 69 points)

|    | <u>Model</u> | <u>ko (ppm/ppm-hr)</u> | <u>K (ppm)</u> | <u>Avg (t-tcalc)^2</u> |
|----|--------------|------------------------|----------------|------------------------|
| 1) | M3           | 0.270413               | 13.58608       | 39                     |
| 2) | M2           | 0.264992               | 12.83308       | 40                     |
| 3) | Z2           | 0.196391               | -              | 269                    |
| 4) | Z1           | 0.207140               | -              | 345                    |
| 5) | F2           | 0.005983               | -              | 1459                   |
| 6) | F1           | 0.004765               | -              | 3684                   |

Percent error in rate constants for M2 and M3:

|    | <u>ko</u> | <u>K</u> |
|----|-----------|----------|
| M2 | -4.68%    | -16.12%  |
| M3 | -2.73%    | -11.20%  |

Experiment D: 100 ppm  $\rightarrow$  10 ppm (61-0 = 61 points)

|    | <u>Model</u> | <u>ko (ppm/ppm-hr)</u> | <u>K (ppm)</u> | <u>Avg (t-tcalc)^2</u> |
|----|--------------|------------------------|----------------|------------------------|
| 1) | M3           | 0.278158               | 15.29156       | 22                     |
| 2) | M2           | 0.267475               | 13.46037       | 24                     |
| 3) | Z2           | 0.205794               | -              | 116                    |
| 4) | Z1           | 0.213314               | -              | 144                    |
| 5) | F2           | 0.005009               | -              | 725                    |
| 6) | F1           | 0.004161               | -              | 1808                   |

Percent error in rate constants for M2 and M3:

|    | <u>ko</u> | <u>K</u> |
|----|-----------|----------|
| M2 | -3.79%    | -12.02%  |
| M3 | +0.06%    | - 0.06%  |

Experiment E: 100 ppm  $\rightarrow$  25 ppm (47-0 = 47 points)

|    | <u>Model</u> | <u>ko (ppm/ppm-hr)</u> | <u>K (ppm)</u> | <u>Avg (t-tcalc)^2</u> |
|----|--------------|------------------------|----------------|------------------------|
| 1) | M3           | 0.266653               | 12.16970       | 23.4                   |
| 2) | M2           | 0.252919               | 9.092224       | 24.6                   |
| 3) | Z2           | 0.219454               | -              | 33.6                   |
| 4) | Z1           | 0.221753               | -              | 35.1                   |
| 5) | F2           | 0.003979               | -              | 236.4                  |
| 6) | F1           | 0.003479               | -              | 546.4                  |

Percent error in rate constants for M2 and M3:

|    | <u>ko</u> | <u>K</u> |
|----|-----------|----------|
| M2 | -9.02%    | -40.57%  |
| M3 | -4.08%    | -20.46%  |

Experiment F: 25 ppm  $\rightarrow$  0.1 ppm (54-4 = 50 points)

|    | <u>Model</u> | <u>ko (ppm/ppm-hr)</u> | <u>K (ppm)</u> | <u>Avg (t-tcalc)^2</u> |
|----|--------------|------------------------|----------------|------------------------|
| 1) | M3           | 0.129580               | 4.971184       | 2197                   |
| 2) | M2           | 0.180118               | 7.698579       | 2312                   |
| 3) | Z2           | 0.072288               | -              | 3093                   |
| 4) | F2           | 0.013911               | -              | 3185                   |
| 5) | Z1           | 0.094949               | -              | 3771                   |
| 6) | F1           | 0.011448               | -              | 3897                   |

Percent error in rate constants for M2 and M3:

|    | <u>ko</u> | <u>K</u> |
|----|-----------|----------|
| M2 | -35.2%    | -47.9%   |
| M3 | -53.4%    | -67.5%   |

Experiment G: 25 ppm  $\rightarrow$  1 ppm (37-0 = 37 points)

|    | <u>Model</u> | <u>ko (ppm/ppm-hr)</u> | <u>K (ppm)</u> | <u>Avg (t-tcalc)<sup>2</sup></u> |
|----|--------------|------------------------|----------------|----------------------------------|
| 1) | M3           | 0.253176               | 13.46697       | 339                              |
| 2) | M2           | 0.300267               | 17.04119       | 343                              |
| 3) | F2           | 0.012084               | -              | 442                              |
| 4) | F1           | 0.010882               | -              | 546                              |
| 5) | Z2           | 0.098019               | -              | 633                              |
| 6) | Z1           | 0.118861               | -              | 844                              |

Percent error in rate constants for M2 and M3:

|    | <u>ko</u> | <u>K</u> |
|----|-----------|----------|
| M2 | +8.01     | +11.38%  |
| M3 | -8.93%    | -11.98%  |

Case 2: Ideal S vs. t data from page F-4 for variable-biomass behavior modified to include the corresponding random error correction terms from page F-6.\*

Experiment A: 100 ppm  $\rightarrow$  0.1 ppm (100-1 = 99 points)

|    | <u>Model</u> | <u>ko (ppm/ppm-hr)</u> | <u>K (ppm)</u> | <u>Avg (t-tcalc)<sup>2</sup></u> |
|----|--------------|------------------------|----------------|----------------------------------|
| 1) | MV           | 0.298088               | 22.06903       | 7.1                              |
| 2) | ZV           | 0.226277               | -              | 8.8                              |
| 3) | FV           | 0.003423               | -              | 23.1                             |

Percent error in rate constants for MV:

% error in ko = +7.23%  
 % error in K = +44.24%

\* All points within the given S range which result in positive values of S (upon incorporating the random error terms) are included.

Experiment B: 100 ppm  $\rightarrow$  1 ppm (94-0 = 94 points)

|    | <u>Model</u> | <u>ko (ppm/ppm-hr)</u> | <u>K (ppm)</u> | <u>Avg (t-tcalc)^2</u> |
|----|--------------|------------------------|----------------|------------------------|
| 1) | MV           | 0.295849               | 21.21199       | 7.4                    |
| 2) | ZV           | 0.230337               | -              | 8.2                    |
| 3) | FV           | 0.003197               | -              | 17.3                   |

Percent error in rate constants for MV:

% error in ko = +6.44%  
 % error in K = +38.64%

Experiment C: 100 ppm  $\rightarrow$  5 ppm (89-0 = 89 points)

|    | <u>Model</u> | <u>ko (ppm/ppm-hr)</u> | <u>K (ppm)</u> | <u>Avg (t-tcalc)^2</u> |
|----|--------------|------------------------|----------------|------------------------|
| 1) | MV           | 0.298154               | 21.99877       | 7.8                    |
| 2) | ZV           | 0.233401               | -              | 8.2                    |
| 3) | FV           | 0.003004               | -              | 13.2                   |

Percent error in rate constants for MV:

% error in ko = +7.25%  
 % error in K = +43.78%

Experiment D: 100 ppm  $\rightarrow$  10 ppm (86-0 = 86 points)

|    | <u>Model</u> | <u>ko (ppm/ppm-hr)</u> | <u>K (ppm)</u> | <u>Avg (t-tcalc)^2</u> |
|----|--------------|------------------------|----------------|------------------------|
| 1) | MV           | 0.318803               | 29.43962       | 8.0                    |
| 2) | ZV           | 0.234781               | -              | 8.4                    |
| 3) | FV           | 0.002887               | -              | 10.7                   |

Percent error in rate constants for MV:

% error in ko = +14.68%  
 % error in K = +92.42%

Experiment E: 100 ppm  $\rightarrow$  25 ppm (80-0 = 80 points)

|    | <u>Model</u> | <u>ko (ppm/ppm-hr)</u> | <u>K (ppm)</u> | <u>Avg (t-tcalc)^2</u> |
|----|--------------|------------------------|----------------|------------------------|
| 1) | MV           | 0.390794               | 56.02126       | 8.6                    |
| 2) | ZV           | 0.237064               | -              | 8.9                    |
| 3) | FV           | 0.002755               | -              | 9.2                    |

Percent error in rate constants for MV:

% error in ko = +40.57%  
 % error in K = +266.15%

Experiment F: 25 ppm  $\rightarrow$  0.1 ppm (21-1 = 20 points)\*

|    | <u>Model</u> | <u>ko (ppm/ppm-hr)</u> | <u>K (ppm)</u> | <u>Avg (t-tcalc)^2</u> |
|----|--------------|------------------------|----------------|------------------------|
| 1) | M3           | 10.43156               | 12.01492       | 0.54                   |
| 2) | MV           | 0.267794               | 18.44074       | 0.55                   |
| 3) | M2           | 10.58294               | 12.23708       | 0.55                   |
| 4) | FV           | 0.009885               | -              | 0.70                   |
| 5) | F2           | 0.517383               | -              | 0.81                   |
| 6) | F1           | 0.520679               | -              | 0.84                   |
| 7) | Z2           | 3.379951               | -              | 1.09                   |
| 8) | Z1           | 4.447615               | -              | 1.15                   |
| 9) | ZV           | 0.090448               | -              | 1.19                   |

Percent error in rate constants for MV:

% error in ko = -3.67%  
 % error in K = +20.53%

\* Bo for this case equals  $(1 + 0.568 (100-25))$  ppm or 46.3 ppm.